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Preface

Numerical Analysis 2000 Vol. II: Interpolation and extrapolation

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This volume is dedicated to two closely related subjects: interpolation and extrapolation. The papers can be divided into three categories: historical papers, survey papers and papers presenting new developments.

Interpolation is an old subject since, as noticed in the paper by M. Gasca and T. Sauer, the term was coined by John Wallis in 1655. Interpolation was the first technique for obtaining an approximation of a function. Polynomial interpolation was then used in quadrature methods and methods for the numerical solution of ordinary differential equations.

Obviously, some applications need interpolation by functions more complicated than polynomials.

The case of rational functions with prescribed poles is treated in the paper by G. Mühlbach. He gives a survey of interpolation procedures using Cauchy–Vandermonde systems. The well-known formulae of Lagrange, Newton and Neville–Aitken are generalized. The construction of rational B-splines is discussed.

Trigonometric polynomials are used in the paper by T. Strohmer for the reconstruction of a signal from non-uniformly spaced measurements. They lead to a well-posed problem that preserves some important structural properties of the original infinite dimensional problem.

More recently, interpolation in several variables was studied. It has applications in finite differences and finite elements for solving partial differential equations. Following the pioneer works of P. de Casteljaou and P. Bézier, another very important domain where multivariate interpolation plays a fundamental role is computer-aided geometric design (CAGD) for the approximation of surfaces.

The history of multivariate polynomial interpolation is related in the paper by M. Gasca and T. Sauer.

The paper by R.A. Lorentz is devoted to the historical development of multivariate Hermite interpolation by algebraic polynomials.

In his paper, G. Walz treats the approximation of multivariate functions by multivariate Bernstein polynomials. An asymptotic expansion of these polynomials is given and then used for building, by extrapolation, a new approximation method which converges much faster.

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Extrapolation is based on interpolation. In fact, extrapolation consists of interpolation at a point outside the interval containing the interpolation points. Usually, this point is either zero or infinity. Extrapolation is used in numerical analysis to improve the accuracy of a process depending of a parameter or to accelerate the convergence of a sequence. The most well-known extrapolation processes are certainly Romberg's method for improving the convergence of the trapezoidal rule for the computation of a definite integral and Aitken's Δ^2 process which can be found in any textbook of numerical analysis.

An historical account of the development of the subject during the 20th century is given in the paper by C. Brezinski.

The theory of extrapolation methods lays on the solution of the system of linear equations corresponding to the interpolation conditions. In their paper, M. Gasca and G. Mühlbach show, by using elimination techniques, the connection between extrapolation, linear systems, totally positive matrices and CAGD.

There exist many extrapolation algorithms. From a finite section S_n, \dots, S_{n+k} of the sequence (S_n) , they built an improved approximation of its limit S . This approximation depends on n and k . When at least one of these indexes goes to infinity, a new sequence is obtained with, possibly, a faster convergence.

In his paper, H.H.H. Homeier studies scalar Levin-type acceleration methods. His approach is based on the notion of remainder estimate which allows to use asymptotic information on the sequence to built an efficient extrapolation process.

The most general extrapolation process known so far is the sequence transformation known under the name of E -algorithm. It can be implemented by various recursive algorithms. In his paper, N. Osada proved that the E -algorithm is mathematically equivalent to the Ford–Sidi algorithm. A slightly more economical algorithm is also proposed.

When S depends on a parameter t , some applications need the evaluation of the derivative of S with respect to t . A generalization of Richardson extrapolation process for treating this problem is considered in the paper by A. Sidi.

Instead of being used for estimating the limit S of a sequence from S_n, \dots, S_{n+k} , extrapolation methods can also be used for predicting the next unknown terms $S_{n+k+1}, S_{n+k+2}, \dots$. The prediction properties of some extrapolation algorithms are analyzed in the paper by E.J. Weniger.

Quite often in numerical analysis, sequences of vectors have to be accelerated. This is, in particular, the case in iterative methods for the solution of systems of linear and nonlinear equations.

Vector acceleration methods are discussed in the paper by K. Jbilou and H. Sadok. Using projectors, they derive a different interpretation of these methods and give some theoretical results. Then, various algorithms are compared when used for the solution of large systems of equations coming out from the discretization of partial differential equations.

Another point of view is taken in the paper by P.R. Graves-Morris, D.E. Roberts and A. Salam. After reminding, in the scalar case, the connection between the ε -algorithm, Padé approximants and continued fractions, these authors show that the vector ε -algorithm is the best all-purpose algorithm for the acceleration of vector sequences.

There is a subject which can be related either to interpolation (more precisely, Hermite interpolation by a rational function at the point zero) and to convergence acceleration: it is Padé approximation. Padé approximation is strongly connected to continued fractions, one of the oldest subject in mathematics since Euclid g.c.d. algorithm is an expansion into a terminating continued fraction.

Although they were implicitly known before, Padé approximants were really introduced by Johan Heinrich Lambert in 1758 and Joseph Louis Lagrange in 1776. Padé approximants have important applications in many branches of applied sciences when the solution of a problem is obtained as a power series expansion and some of its properties have to be guessed from its first Taylor coefficients. In this volume, two papers deal with nonclassical applications of Padé approximation.

M. Prévost shows how Padé approximants can be used to obtain Diophantine approximations of real and complex numbers and then proving irrationality. Padé approximation of the asymptotic expansion of the remainder of a series also provides Diophantine approximations.

The solution of a discrete dynamical system can be related to matrix Hermite–Padé approximants, an approach developed in the paper by V. Sorokin and J. van Iseghem. Spectral properties of the band operator are investigated. The inverse spectral method is used for the solution of dynamical systems defined by a Lax pair.

Obviously, all aspects of interpolation and extrapolation have not been treated in this volume. However, many important topics have been covered.

I would like to thank all authors for their efforts.



Convergence acceleration during the 20th century

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1. Introduction

In numerical analysis many methods produce sequences, for instance iterative methods for solving systems of equations, methods involving series expansions, discretization methods (that is methods depending on a parameter such that the approximate solution tends to the exact one when the parameter tends to zero), perturbation methods, etc. Sometimes, the convergence of these sequences is slow and their effective use is quite limited. Convergence acceleration methods consist of transforming a slowly converging sequence (S_n) into a new sequence (T_n) converging to the same limit faster than the initial one. Among such *sequence transformations*, the most well known are certainly Richardson's extrapolation algorithm and Aitken's Δ^2 process. All known methods are constructed by extrapolation and they are often called *extrapolation methods*. The idea consists of interpolating the terms $S_n, S_{n+1}, \dots, S_{n+k}$ of the sequence to be transformed by a sequence satisfying a certain relationship depending on parameters. This set of sequences is called *kernel* of the transformation and every sequence of this set is transformed into a constant sequence by the transformation into consideration. For example, as we will see below, the kernel of Aitken's Δ^2 process is the set of sequences satisfying $\forall n, a_0(S_n - S) + a_1(S_{n+1} - S) = 0$, where a_0 and a_1 are parameters such that $a_0 + a_1 \neq 0$. If Aitken's process is applied to such a sequence, then the constant sequence $(T_n = S)$ is obtained. The parameters involved in the definition of the kernel are uniquely determined by the interpolation conditions and then the limit of the interpolating sequence of the kernel is taken as an approximation of the limit of the sequence to be accelerated. Since this limit depends on the index n , it will be denoted by T_n . Effectively, the sequence (S_n) has been transformed into a new sequence (T_n) .

This paper, which is based on [31], but includes new developments obtained since 1995, presents my personal views on the historical development of this subject during the 20th century. I do not pretend to be exhaustive nor even to quote every important contribution (if a reference does not

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appear below, it does not mean that it is less valuable). I refer the interested reader to the literature and, in particular to the recent books [55,146,33,144]. For an extensive bibliography, see [28].

I will begin with scalar sequences and then treat the case of vector ones. As we will see, a sequence transformation able to accelerate the convergence of *all* scalar sequences cannot exist. Thus, it is necessary to obtain many different convergence acceleration methods, each being suitable for a particular class of sequences. Many authors have studied the properties of these procedures and proved some important classes of sequences to be accelerable by a given algorithm. Scalar sequence transformations have also been extensively studied from the theoretical point of view.

The situation is more complicated and more interesting for vector sequences. In the case of a sequence of vectors, it is always possible to apply a scalar acceleration procedure componentwise. However, such a strategy does not take into account connections which may exist between the various components, as in the important case of sequences arising from iterative methods for solving a system of linear or nonlinear equations.

2. Scalar sequences

Let (S_n) be a scalar sequence converging to a limit S . As explained above, an extrapolation method consists of transforming this sequence into a new one, (T_n) , by a sequence transformation $T: (S_n) \rightarrow (T_n)$. The transformation T is said to *accelerate the convergence* of the sequence (S_n) if and only if

$$\lim_{n \rightarrow \infty} \frac{T_n - S}{S_n - S} = 0.$$

We can then say that (T_n) converges (to S) *faster than* (S_n) .

The first methods to have been used were linear transformations

$$T_n = \sum_{i=0}^{\infty} a_{ni} S_i, \quad n = 0, 1, \dots,$$

where the numbers a_{ni} are constants independent of the terms of the sequence (S_n) . Such a linear transformation is usually called a *summation process* and its properties are completely determined by the matrix $A = (a_{ni})$. For practical reasons, only a finite number of the coefficients a_{ni} are different from zero for each n . Among such processes are those named after Euler, Cesaro and Hölder. In the case of linear methods, the convergence of the sequence (T_n) to S for any converging sequence (S_n) is governed by the Toeplitz summability theorem; see [115] for a review. Examples of such processes are

$$T_n = \frac{1}{n+1} \sum_{i=0}^n S_i$$

or

$$T_n = \frac{1}{k+1} \sum_{i=n}^{n+k} S_i.$$

In the second case, the sequence (T_n) also depends on a second index, k , and the convergence has to be studied either when k is fixed and n tends to infinity, or when n is fixed and k tends to infinity.

With respect to convergence acceleration, summation processes are usually only able to accelerate the convergence of restricted classes of sequences and this is why the numerical analysts of the 20th century turned their efforts to nonlinear transformations. However, there is one exception: Richardson's extrapolation process.

2.1. Richardson's process

It seems that the first appearance of a particular case of what is now called the Richardson extrapolation process is due to Christian Huygens (1629–1695). In 1903, Robert Moir Milne (1873) applied the idea of Huygens for computing π [101]. The same idea was exploited again by Karl Kommerell (1871–1948) in his book of 1936 [78]. As explained in [143], Kommerell can be considered as the real discoverer of Romberg's method although he used this scheme in the context of approximating π .

Let us now come to the procedures used for improving the accuracy of the trapezoidal rule for computing approximations to a definite integral. In the case of a sufficiently smooth function, the error of this method is given by the Euler–Maclaurin expansion. In 1742, Colin Maclaurin (1698–1746) [90] showed that its precision could be improved by forming linear combinations of the results obtained with various stepsizes. His procedure can be interpreted as a preliminary version of Romberg's method; see [49] for a discussion.

In 1900, William Fleetwood Sheppard (1863–1936) used an elimination strategy in the Euler–Maclaurin quadrature formula with $h_n = r_n h$ and $1 = r_0 < r_1 < r_2 < \dots$ to produce a better approximation to the given integral [132].

In 1910, combining the results obtained with the stepsizes h and $2h$, Lewis Fry Richardson (1881–1953) eliminated the first term in a discretization process using central differences [119]. He called this procedure the *deferred approach to the limit* or h^2 -extrapolation. The transformed sequence (T_n) is given by

$$T_n = \frac{h_{n+1}^2 S(h_n) - h_n^2 S(h_{n+1})}{h_{n+1}^2 - h_n^2}.$$

In a 1927 paper [120] he used the same technique to solve a 6th order differential eigenvalue problem. His process was called (h^2, h^4) -extrapolation. Richardson extrapolation consists of computing the value at 0, denoted by $T_k^{(n)}$, of the interpolation polynomial of the degree at most k , which passes through the points $(x_n, S_n), \dots, (x_{n+k}, S_{n+k})$. Using the Neville–Aitken scheme for these interpolation polynomials, we immediately obtain

$$T_{k+1}^{(n)} = \frac{x_{n+k+1} T_k^{(n)} - x_n T_k^{(n+1)}}{x_{n+k+1} - x_n}$$

with $T_0^{(n)} = S_n$.

Let us mention that Richardson referred to a 1926 paper by Nikolai Nikolaevich Bogolyubov (born in 1909) and Nikolai Mitrofanovich Krylov (1879–1955) where the procedure (often called the *deferred approach to the limit*) can already be found [11].

In 1955, Werner Romberg (born in 1909) was the first to use repeatedly an elimination approach for improving the accuracy of the trapezoidal rule [121]. He himself refers to the book of Lothar Collatz (1910–1990) of 1951 [50]. The procedure became widely known after the rigorous error

analysis given in 1961 by Friedrich L. Bauer [3] and the work of Eduard L. Stiefel (1909–1978) [138]. Romberg's derivation of his process was heuristic. It was proved by Pierre-Jean Laurent in 1963 [81] that the process comes out from the Richardson process by choosing $x_n = h_n^2$ and $h_n = h_0/2^n$. Laurent also gave conditions on the choice of the sequence (x_n) in order that the sequences $(T_k^{(n)})$ tend to S either when k or n tends to infinity. Weaker conditions were given by Michel Crouzeix and Alain L. Mignot in [52, pp. 52–55]. As we shall see below, extensions of Romberg's method to nonsmooth integrands leads to a method called the E -algorithm.

Applications of extrapolation to the numerical solution of ordinary differential equations were studied by H.C. Bolton and H.I. Scoins in 1956 [12], Roland Bulirsch and Josef Stoer in 1964–1966 [47] and William B. Gragg [65] in 1965. The case of difference methods for partial differential equations was treated by Guriĭ Ivanovich Marchuk and V.V. Shaidurov [91]. Sturm–Liouville problems are discussed in [117]. Finally, we mention that Heinz Rutishauser (1918–1970) pointed out in 1963 [122] that Romberg's idea can be applied to any sequence as long as the error has an asymptotic expansion of a form similar to the Euler–Maclaurin's.

For a detailed history of the Richardson method, its developments and applications, see [57,77,143].

2.2. Aitken's process and the ε -algorithm

The most popular nonlinear acceleration method is certainly Aitken's A^2 process which is given by

$$T_n = \frac{S_n S_{n+2} - S_{n+1}^2}{S_{n+2} - 2S_{n+1} + S_n} = S_n - \frac{(S_{n+1} - S_n)^2}{S_{n+2} - 2S_{n+1} + S_n}, \quad n = 0, 1, \dots$$

The method was stated by Alexander Craig Aitken (1895–1967) in 1926 [1], who used it to accelerate the convergence of Bernoulli's method for computing the dominant zero of a polynomial. Aitken pointed out that the same method was obtained by Hans von Naegelsbach (1838) in 1876 in his study of Furstenau's method for solving nonlinear equations [104]. The process was also given by James Clerk Maxwell (1831–1879) in his *Treatise on Electricity and Magnetism* of 1873 [95]. However, neither Naegelsbach nor Maxwell used it for the purpose of acceleration. Maxwell wanted to find the equilibrium position of a pointer oscillating with an exponentially damped simple harmonic motion from three experimental measurements. It is surprising that Aitken's process was known to Takakazu Seki (1642–1708), often considered the greatest Japanese mathematician. In his book *Katsuyō Sanpō*, Vol. IV, he used this process to compute the value of π , the length of a chord and the volume of a sphere. This book was written around 1680 but only published in 1712 by his disciple Murahide Araki. Parts of it can be found in [73]. Let us mention that the Japanese characters corresponding to Takakazu have another pronunciation which is Kōwa. This is the reason why this mathematician is often called, erroneously as in [29,31] Seki Kōwa.

What makes Aitken's process so popular is that it accelerates the convergence of all linearly converging sequences, that is sequences such that $\exists a \neq 1$

$$\lim_{n \rightarrow \infty} \frac{S_{n+1} - S}{S_n - S} = a.$$

It can even accelerate some logarithmic sequences (that is corresponding to $a = 1$) which are those with the slowest convergence and the most difficult to accelerate.

Aitken’s Δ^2 process is exact (which means that $\forall n, T_n = S$) for sequences satisfying, $a_0(S_n - S) + a_1(S_{n+1} - S) = 0, \forall n, a_0 a_1 \neq 0, a_0 + a_1 \neq 0$. Such sequences form the kernel of Aitken’s process. The idea naturally arose of finding a transformation with the kernel

$$a_0(S_n - S) + \dots + a_k(S_{n+k} - S) = 0, \quad \forall n,$$

$a_0 a_k \neq 0, a_0 + \dots + a_k \neq 0$. A particular case of $k = 2$ was already treated by Maxwell in his book of 1873 and a particular case of an arbitrary value of k was studied by T.H. O’Beirne in 1947 [107]. This last work remains almost unknown since it was published only as an internal report. The problem was handled in full generality by Daniel Shanks (1917–1996) in 1949 [130] and again in 1955 [131]. He obtained the sequence transformation defined by

$$T_n = e_k(S_n) = \frac{\begin{vmatrix} S_n & S_{n+1} & \dots & S_{n+k} \\ S_{n+1} & S_{n+2} & \dots & S_{n+k+1} \\ \vdots & \vdots & & \vdots \\ S_{n+k} & S_{n+k+1} & \dots & S_{n+2k} \end{vmatrix}}{\begin{vmatrix} \Delta^2 S_n & \dots & \Delta^2 S_{n+k-1} \\ \vdots & & \vdots \\ \Delta^2 S_{n+k-1} & \dots & \Delta^2 S_{n+2k-2} \end{vmatrix}}.$$

When $k = 1$, Shanks transformation reduces to the Aitken’s Δ^2 process. It can be proved that $e_k(S_n) = S, \forall n$ if and only if (S_n) belongs to the kernel of the transformation given above. The same ratios of determinants were obtained by R.J. Schmidt in 1941 [127] in his study of a method for solving systems of linear equations.

The determinants involved in the definition of $e_k(S_n)$ have a very special structure. They are called *Hankel determinants* and were studied by Hermann Hankel (1839–1873) in his thesis in 1861 [72]. Such determinants satisfy a five-term recurrence relationship. This relation was used by O’Beirne and Shanks to implement the transformation by computing separately the numerators and the denominators of the $e_k(S_n)$ ’s. However, numerical analysts know it is difficult to compute determinants (too many arithmetical operations are needed and rounding errors due to the computer often lead to a completely wrong result). A recursive procedure for computing the $e_k(S_n)$ ’s without computing the determinants involved in their definition was needed. This algorithm was obtained in 1956 by Peter Wynn. It is called the ε -algorithm [147]. It is as follows. One starts with

$$\varepsilon_{-1}^{(n)} = 0, \quad \varepsilon_0^{(n)} = S_n$$

and then

$$\varepsilon_{k+1}^{(n)} = \varepsilon_{k-1}^{(n+1)} + \frac{1}{\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}}.$$

Note that the numbers $\varepsilon_k^{(n)}$ ’s fill out a two-dimensional array. The ε -algorithm is related to Shanks transformation by

$$\varepsilon_{2k}^{(n)} = e_k(S_n) \quad \text{and} \quad \varepsilon_{2k+1}^{(n)} = 1/e_k(\Delta S_n).$$

Thus, the ε ’s with an odd lower index are only auxiliary quantities. They can be eliminated from the algorithm, thus leading to the so-called *cross rule* due to Wynn [153].

When implementing the ε -algorithm or using Wynn's cross rule, division by zero can occur and the algorithm must be stopped. However, if the singularity is confined, a term that will again be used in Section 1.6, that is if it occurs only for some adjacent values of the indexes k and n , one may jump over it by using *singular rules* and continue the computation. If a division by a number close to zero arises, the algorithm becomes numerically unstable due to the cancellation errors. A similar situation holds for the other convergence acceleration algorithms. The study of such problems was initiated by Wynn in 1963 [151], who proposed particular rules for the ε -algorithm which are more stable than the usual rules. They were extended by Florent Cordellier in 1979 [51,151]. Particular rules for the θ -algorithm were obtained by Redivo Zaglia [155].

The convergence and acceleration properties of the ε -algorithm have only been completely described only for two classes of sequences, namely totally monotonic and totally oscillating sequences [154,15,16].

Shanks' transformation and the ε -algorithm have close connections to Padé approximants, continued fractions and formal orthogonal polynomials; see, for example [18].

2.3. Subsequent developments

The Shanks transformation and the ε -algorithm sparked the rebirth of the study of nonlinear acceleration processes. They now form an independent chapter in numerical analysis with connections to other important topics such as orthogonal and biorthogonal polynomials, continued fractions, and Padé approximants. They also have applications to the solution of systems of linear and nonlinear equations, the computation of the eigenvalues of a matrix, the solution of systems of linear and nonlinear equations, and many other topics, see [40]. Among other acceleration methods which were obtained and studied, are the W -process of Samuel Lubkin [89], the method of Kjell J. Overholt [110], the ρ -algorithm of Wynn [148], the G -transformation of H.L. Gray, T.A. Atchison and G.V. McWilliams [70], the θ -algorithm of Claude Brezinski [14], the transformations of Bernard Germain-Bonne [63] and the various transformations due to David Levin [85]. To my knowledge, the only known acceleration theorem for the ρ -algorithm was obtained by Naoki Osada [108]. Simultaneously, several applications began to appear. For example, the ε -algorithm provides a quadratically convergent method for solving systems of nonlinear equations and it does not require the knowledge of any derivative. This procedure was proposed simultaneously by Brezinski [13] and Eckhart Gekeler [61]. It has important applications to the solution of boundary value problems for ordinary differential equations [44]. Many other algorithms are given in the work of Ernst Joachim Weniger [145], which also contains applications to physics, or in the book of Brezinski and Michela Redivo Zaglia [40] where applications to various domains of numerical analysis can be found. The authors of this book provide FORTRAN subroutines. The book of Annie Cuyt and Luc Wuytack must also be mentioned [53]. The ε -algorithm has been applied to statistics, see the work of Alain Berline [9], and to the acceleration of the convergence of sequences of random variables, considered by Hélène Lavastre [82]. Applications to optimization were proposed by Le Ferrand [84] and Bouchta Rhanizar [118].

Instead of using a quite complicated algorithm, such as the ε -algorithm, it can be interesting to use a simpler one (for instance, Aitken's A^2 process) iteratively. Such a use consists of applying the algorithm to (S_n) to produce a new sequence (T_n) , then to apply the same algorithm to (T_n) , and so on. For example, applying the iterated A^2 process to the successive convergents

of a periodic continued fraction produces a better acceleration than using the ε -algorithm [24]. In particular, the iterated Δ^2 process transforms a logarithmic sequence into a sequence converging linearly and linear convergence into superlinear, to my knowledge the only known cases of such transformations.

The experience gained during these years lead to a deeper understanding of the subject. Research workers began to study more theoretical and general questions related to the theory of convergence acceleration. The first attempt was made by R. Pennacchi in 1968 [114], who studied rational sequence transformations. His work was generalized by Germain–Bonne in 1973 [62], who proposed a very general framework and showed how to construct new algorithms for accelerating some classes of sequences. However, a ground breaking discovery was made by Jean Paul Delahaye and Germain–Bonne in 1980 [56]. They proved that if a set of sequences satisfies a certain property, called *remanence* (too technical to be explained here), then a universal algorithm, i.e. one able to accelerate *all* sequences of this set, cannot exist. This result shows the limitations of acceleration methods. Many sets of sequences were proved to be remanent, for example, the sets of monotonic or logarithmic sequences. Even some subsets of the set of logarithmic sequences are remanent.

Moulay Driss Benchiboun [5] observed that all the sequence transformations found in the literature could be written as

$$T_n = \frac{f(S_n, \dots, S_{n+k})}{Df(S_n, \dots, S_{n+k})}$$

with $D^2 f \equiv 0$, where Df denotes the sum of the partial derivatives of the function f . The reason for that fact was explained by Brezinski [26], who showed that it is related to the translativity property of sequence transformations. Hassane Sadok [123] extended these results to the vector case. Abderrahim Benazzouz [7] proved that quasilinear transformations can be written as the composition of two projections.

In many transformations, such as Shanks', the quantities computed are expressed as a ratio of determinants. This property is related to the existence of a triangular recurrence scheme for their computation as explained by Brezinski and Guido Walz [46].

Herbert Homeier [74] studied a systematic procedure for constructing sequences transformations. He considered iterated transformations which are *hierarchically consistent*, which means that the kernel of the basic transformation is the lowest one in the hierarchy. The application of the basic transformation to a sequence which is higher in the hierarchy leads to a new sequence belonging to a kernel lower in the hierarchy. Homeier wrote several papers on this topics.

Thus, the theory of convergence acceleration methods has progressed impressively. The practical side was not forgotten and authors obtained a number of special devices for improving their efficiency. For example, when a certain sequence is to be accelerated, it is not obvious to know in advance which method will give the best result unless some properties of the sequence are already known. Thus, Delahaye [54] proposed using simultaneously several transformations and selecting, at each step of the procedure, one answer among the answers provided by the various algorithms. He proved that, under some assumptions, some tests are able to find automatically the best answer. The work of Delahaye was extended by Abdelhak Fdil [58,59]. The various answers could also be combined leading to *composite* transformations [23]. It is possible, in some cases, to extract a linear subsequence from the original one and then to accelerate it, for example, by Aitken's Δ^2 process [37]. Devices for controlling the error were also constructed [21].

When faced with the problem of accelerating the convergence of a given sequence, two approaches are possible. The first is to use a known extrapolation procedure and to try to prove that it accelerates the convergence of the given sequence. The second possibility is to construct an extrapolation procedure especially for that sequence. Convergence tests for sequences and series can be used for that purpose as explained by Brezinski [25]. This approach was mostly developed by Ana Cristina Matos [92]. Special extrapolation procedures for sequences such that $\forall n, S_n - S = a_n D_n$, where (D_n) is a known sequence and (a_n) an unknown one, can also be constructed from the asymptotic properties of the sequences (a_n) and (D_n) . Brezinski and Redivo Zaglia did this in [39].

A.H. Bentbib [10] considered the acceleration of sequences of intervals. Mohammed Senhadji [129] defined and studied the condition number of a sequence transformation.

2.4. The E -algorithm

As we see above, the quantities involved in Shanks transformation are expressed as a ratio of determinants and the ε -algorithm allows one to compute them recursively. It is well known that an interpolation polynomial can be expressed as a ratio of determinants. Thus polynomial extrapolation also leads to such a ratio and the Neville–Aitken scheme can be used to avoid the computation of these determinants which leads to the Richardson extrapolation algorithm. A similar situation arises for many other transformations: in each case, the quantities involved are expressed as a ratio of special determinants and, in each case, one seeks for a special recursive algorithm for the practical implementation of the transformation. Thus, there was a real need for a general theory of such sequence transformations and for a single general recursive algorithm for their implementation. This work was performed independently between 1973 and 1980 by five different people. It is now known as the E -algorithm.

It seems that the first appearance of this algorithm is due to Claus Schneider in a paper received on December 21, 1973 [128]. The quantities $S(h_i)$ being given for $i = 0, 1, \dots$, Schneider looked for $S'(h) = S' + a_1 g_1(h) + \dots + a_k g_k(h)$ satisfying the interpolation conditions $S'(h_i) = S(h_i)$ for $i = n, \dots, n+k$, where the g_j 's are given functions of h . Of course, the value of the unknown S' thus obtained will depend on the indexes k and n . Assuming that $\forall j, g_j(0) = 0$, we have $S' = S'(0)$. Denoting by ϕ_k^n the extrapolation functional on the space of functions f defined at the points $h_0 > h_1 > \dots > 0$ and at the point 0 and such that $\phi_k^n f = f(0)$, we have

$$\phi_k^n S' = c_0 S(h_n) + \dots + c_k S(h_{n+k})$$

with $c_0 + \dots + c_k = 1$. The interpolation conditions become

$$\phi_k^n E = 1, \quad \text{and} \quad \phi_k^n g_j = 0, \quad j = 1, \dots, k$$

with $E(h) \equiv 1$. Schneider wanted to express the functional ϕ_k^n in the form $\phi_k^n = a\phi_{k-1}^n + b\phi_{k-1}^{n+1}$. He obtained the two conditions

$$\phi_k^n E = a + b = 1$$

and

$$\phi_k^n g_k = a\phi_{k-1}^n g_k + b\phi_{k-1}^{n+1} g_k = 0.$$

The values of a and b follow immediately and we have

$$\phi_k^n = \frac{[\phi_{k-1}^{n+1} g_k] \phi_{k-1}^n - [\phi_{k-1}^n g_k] \phi_{k-1}^{n+1}}{[\phi_{k-1}^{n+1} g_k] - [\phi_{k-1}^n g_k]}.$$

Thus, the quantities $\phi_k^n S'$ can be recursively computed by this scheme. The auxiliary quantities $\phi_k^n g_j$ needed in this formula must be computed separately by the same scheme using a different initialization. As we shall see below, this algorithm is just the *E*-algorithm. In a footnote, Schneider mentioned that this representation for ϕ_k^n was suggested by Börsch–Supan from Johannes Gutenberg Universität in Mainz.

In 1976, Günter Meinardus and G.D. Taylor wrote a paper [97] on best uniform approximation by functions from $\text{span}(g_1, \dots, g_N) \subset C[a, b]$. They defined the linear functionals L_n^k on $C[a, b]$ by

$$L_n^k(f) = \sum_{i=n}^{n+k} c_i f(h_i),$$

where $a \leq h_1 < h_2 < \dots < h_{N+1} \leq b$ and where the coefficients c_i , which depend on n and k , are such that $c_n > 0, c_i \neq 0$ for $i = n, \dots, n+k$, $\text{sign } c_i = (-1)^{i-n}$ and

$$\sum_{i=n}^{n+k} |c_i| = 1,$$

$$\sum_{i=n}^{n+k} c_i g_j(h_i) = 0, \quad j = 1, \dots, k.$$

By using Gaussian elimination to solve the system of linear equations

$$\sum_{i=n}^N a_i g_i(h_j) + (-1)^j \lambda = f(h_j), \quad j = 1, \dots, k,$$

Meinardus and Taylor obtained a recursive scheme

$$L_i^k(f) = \frac{L_{i+1}^{k-1}(g_k)L_i^{k-1}(f) - L_i^{k-1}(g_k)L_{i+1}^{k-1}(f)}{L_{i+1}^{k-1}(g_k) - L_i^{k-1}(g_k)}$$

with $L_i^0(f) = f(h_i)$, $i = n, \dots, n+k$. This is the same scheme as above.

Newton’s formula for computing the interpolation polynomial is well known. It is based on divided differences. One can try to generalize these formulae to the case of interpolation by a linear combination of functions from a complete Chebyshev system (a technical concept which insures the existence and uniqueness of the solution). We seek

$$P_k^{(n)}(x) = a_0 g_0(x) + \dots + a_k g_k(x),$$

satisfying the interpolation conditions

$$P_k^{(n)}(x_i) = f(x_i), \quad i = n, \dots, n+k,$$

where the x_i ’s are distinct points and the g_i ’s given functions. The $P_k^{(n)}$ can be recursively computed by an algorithm which generalizes the Neville–Aitken scheme for polynomial interpolation. This algorithm was obtained by Günter Mühlbach in 1976 [103] from a generalization of the notion of divided differences and their recurrence relationship. This algorithm was called the Mühlbach–Neville–Aitken algorithm, for short the MNA. It is as follows:

$$P_k^{(n)}(x) = \frac{g_{k-1,k}^{(n+1)}(x)P_{k-1}^{(n)}(x) - g_{k-1,k}^{(n)}(x)P_{k-1}^{(n+1)}(x)}{g_{k-1,k}^{(n+1)}(x) - g_{k-1,k}^{(n)}(x)}$$

with $P_0^{(n)}(x) = f(x_n)g_0(x)/g_0(x_n)$. The $g_{k,i}^{(n)}$'s can be recursively computed by a quite similar relationship

$$g_{k,i}^{(n)}(x) = \frac{g_{k-1,k}^{(n+1)}(x)g_{k-1,i}^{(n)}(x) - g_{k-1,k}^{(n)}(x)g_{k-1,i}^{(n+1)}(x)}{g_{k-1,k}^{(n+1)}(x) - g_{k-1,k}^{(n)}(x)}$$

with $g_{0,i}^{(n)}(x) = g_i(x_n)g_0(x)/g_0(x_n) - g_i(x)$. If $g_0(x) \equiv 1$, if it is assumed that $\forall i > 0, g_i(0) = 0$, the quantities $P_k^{(n)}(0)$ are the same as those obtained by the E -algorithm and the MNA reduces to it. Let us mention that, in fact, the MNA is closely related to the work of Henri Marie Andoyer (1862–1929) which goes back to 1906 [2]; see [30] for detailed explanations.

We now come to the work of Tore Håvie. We already mentioned Romberg's method for accelerating the convergence of the trapezoidal rule. The success of this procedure is based on the existence of the Euler–Maclaurin expansion for the error. This expansion only holds if the function to be integrated has no singularity in the interval. In the presence of singularities, the expansion of the error is no longer a series in h^2 (the stepsize) but a more complicated one depending on the singularity. Thus, Romberg's scheme has to be modified to incorporate the various terms appearing in the expansion of the error. Several authors worked on this question, treating several types of singularities. In particular, Håvie began to study this question under Romberg (Romberg emigrated to Norway and came to Trondheim in 1949). In 1978, Håvie wrote a report, published one year later [71], where he treated the most general case of an error expansion of the form

$$S(h) - S = a_1g_1(h) + a_2g_2(h) + \dots,$$

where $S(h)$ denotes the approximation obtained by the trapezoidal rule with step size h to the definite integral S and the g_i are the known functions (forming an asymptotic sequence when h tends to zero) appearing in the expansion of the error. Let $h_0 > h_1 > \dots > 0$, $S_n = S(h_n)$ and $g_i(n) = g_i(h_n)$. Håvie set

$$E_1^{(n)} = \frac{g_1(n+1)S_n - g_1(n)S_{n+1}}{g_1(n+1) - g_1(n)}.$$

Replacing S_n and S_{n+1} by their expansions, he obtained

$$E_1^{(n)} = S + a_2g_{1,2}^{(n)} + a_3g_{1,3}^{(n)} + \dots$$

with

$$g_{1,i}^{(n)} = \frac{g_1(n+1)g_i(n) - g_1(n)g_i(n+1)}{g_1(n+1) - g_1(n)}.$$

The same process can be repeated for eliminating $g_{1,2}^{(n)}$ in the the expansion of $E_1^{(n)}$, and so on. Thus, once again we obtain the E -algorithm

$$E_k^{(n)} = \frac{g_{k-1,k}^{(n+1)}E_{k-1}^{(n)} - g_{k-1,k}^{(n)}E_{k-1}^{(n+1)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}}$$

with $E_0^{(n)} = S_n$ and $g_{0,i}^{(n)} = g_i(n)$. The auxiliary quantities $g_{k,i}^{(n)}$ are recursively computed by the quite similar rule

$$g_{k,i}^{(n)} = \frac{g_{k-1,k}^{(n+1)}g_{k-1,i}^{(n)} - g_{k-1,k}^{(n)}g_{k-1,i}^{(n+1)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}}$$

with $g_{0,i}^{(n)} = g_i(n)$.

Håvie gave an interpretation of this algorithm in terms of the Gaussian elimination process for solving the system

$$E_k^{(n)} + b_1 g_1(n+i) + \cdots + b_k g_k(n+i) = S_{n+i}, \quad i = 0, \dots, k$$

for the unknown $E_k^{(n)}$.

In 1980, Brezinski took up the same problem, but from the point of view of extrapolation [19]. Let (S_n) be the sequence to be accelerated. Interpolating it by a sequence of the form $S'_n = S + a_1 g_1(n) + \cdots + a_k g_k(n)$, where the g_i 's are known sequences which can depend on the sequence (S_n) itself, leads to

$$S_{n+i} = S'_{n+i}, \quad i = 0, \dots, k.$$

Solving this system directly for the unknown S (which, since it depends on n and k , will be denoted by $E_k^{(n)}$) gives

$$E_k^{(n)} = \frac{\begin{vmatrix} S_n & \cdots & S_{n+k} \\ g_1(n) & \cdots & g_1(n+k) \\ \vdots & & \vdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ g_1(n) & \cdots & g_1(n+k) \\ \vdots & & \vdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}.$$

Thus $E_k^{(n)}$ is given as a ratio of determinants which is very similar to the ratios previously mentioned. Indeed, for the choice $g_i(n) = \Delta S_{n+i}$, the ratio appearing in Shanks transformation results while, when $g_i(n) = x_n^i$, we obtain the ratio expressing the quantities involved in the Richardson extrapolation process. Other algorithms may be similarly derived.

Now the problem is to find a recursive algorithm for computing the $E_k^{(n)}$'s. Applying Sylvester's determinantal identity, Brezinski obtained the two rules of the above E -algorithm. His derivation of the E -algorithm is closely related to Håvie's since Sylvester's identity can be proved by using Gaussian elimination. Brezinski also gave convergence and acceleration results for this algorithm when the $(g_i(n))$ satisfy certain conditions [19]. These results show that, for accelerating the convergence of a sequence, it is necessary to know the expansion of the error $S_n - S$ with respect to some asymptotic sequence $(g_1(n)), (g_2(n)), \dots$. The $g_i(n)$ are those to be used in the E -algorithm. It can be proved that, $\forall k$

$$\lim_{n \rightarrow \infty} \frac{E_{k+1}^{(n)} - S}{E_k^{(n)} - S} = 0.$$

These results were refined by Avram Sidi [134–136]. Thus the study of the asymptotic expansion of the error of the sequences to be accelerated is of primary importance, see Walz [144]. For example, Mohammed Kzaz [79,80] and Pierre Verlinden [142] applied this idea to the problem of accelerating the convergence of Gaussian quadrature formulae [79] and Pedro Lima and Mario Graça to boundary value problems with singularities [88,87] (see also the works of Lima and Diogo [87], and Lima and Carpentier [86]). Other acceleration results were obtained by Matos and Marc Prévost [94], Prévost

[116] and Pascal Mortreux and Prévost [102]. An algorithm, more economical than the E -algorithm, was given by William F. Ford and Avram Sidi [60]. The connection between the E -algorithm and the ε -algorithm was studied by Bernhard Beckermann [4]. A general ε -algorithm connected to the E -algorithm was given by Carsten Carstensen [48]. See [27] for a more detailed review on the E -algorithm.

Convergence acceleration algorithms can also be used for predicting the unknowns terms of a series or a sequence. This idea, introduced by Jacek Gilewicz [64], was studied by Sidi and Levin [137], Brezinski [22] and Denis Vekemans [141].

2.5. A new approach

Over the years, a quite general framework was constructed for the theory of extrapolation algorithms. The situation was quite different for the practical construction of extrapolation algorithms and there was little systematic research in their derivation. However, thanks to a formalism due to Weniger [145], such a construction is now possible, see Brezinski and Matos [38]. It is as follows. Let us assume that the sequence (S_n) to be accelerated satisfies, $\forall n, S_n - S = a_n D_n$ where (D_n) is a known sequence, called a *remainder* (or error) *estimate* for the sequence (S_n) , and (a_n) an unknown sequence. It is possible to construct a sequence transformation such that its kernel is precisely this set of sequences. For that purpose, we have to assume that a difference operator L (that is a linear mapping of the set of sequences into itself) exists such that $\forall n, L(a_n) = 0$. This means that the sequence obtained by applying L to the sequence (a_n) is identically zero. Such a difference operator is called an *annihilation* operator for the sequence (a_n) . We have

$$\frac{S_n}{D_n} - \frac{S}{D_n} = a_n.$$

Applying L and using linearity leads to

$$L\left(\frac{S_n}{D_n}\right) - SL\left(\frac{1}{D_n}\right) = L(a_n) = 0.$$

We solve for S and designate it by the sequence transformation

$$T_n = \frac{L(S_n/D_n)}{L(1/D_n)}.$$

The sequence (T_n) is be such that $\forall n, T_n = S$ if and only if $\forall n, S_n - S = a_n D_n$. This approach is highly versatile.

All the algorithms described above and the related devices such as error control, composite sequence transformations, least squares extrapolation, etc., can be put into this framework. Moreover, many new algorithms can be obtained using this approach. The E -algorithm can also be put into this framework which provides a deeper insight and leads to new properties [41]. Matos [93], using results from the theory of difference equations, obtained new and general convergence and acceleration results when (a_n) has an asymptotic expansion of a certain form.

2.6. Integrable systems

The connection between convergence acceleration algorithms and discrete integrable systems is a subject whose interest is rapidly growing among physicists. When a numerical scheme is used for

integrating a partial differential evolution equation, it is important that it preserves the quantities that are conserved by the partial differential equation itself. An important character is the *integrability* of the equation. Although this term has not yet received a completely satisfactory definition (see [66]), it can be understood as the ability to write the solution explicitly in terms of a finite number of functions or as the confinement of singularities in finite domains. The construction of integrable discrete forms of integrable partial differential equations is highly nontrivial. A major discovery in the field of integrability was the occurrence of a solitary wave (called a *soliton*) in the Korteweg–de Vries (KdV) equation. Integrability is a rare phenomenon and the typical dynamical system is nonintegrable. A test of integrability, called *singularity confinement*, was given by B. Grammaticos, A. Ramani and V. Papageorgiou [67]. It turns out that this test is related to the existence of singular rules for avoiding a division by zero in convergence acceleration algorithms (see Section 1.2).

The literature on this topic is vast and we cannot enter into the details of it. We only want to give an indication of the connection between these two subjects since both domains could benefit from it.

In the rule for the ε -algorithm, V. Papageorgiou, B. Grammaticos and A. Ramani set $m = k + n$ and replaced $\varepsilon_k^{(n)}$ by $u(n, m) + mp + nq$, where p and q satisfy $p^2 - q^2 = 1$. They obtained [111]

$$[p - q + u(n, m + 1) - u(n + 1, m)][p + q + u(n + 1, m + 1) - u(n, m)] = p^2 - q^2.$$

This is the discrete lattice KdV equation. Since this equation is integrable, one can expect integrability to hold also for the ε -algorithm, and, thanks to the singular rules of Wynn and Cordellier mentioned at the end of Subsection 1.2, this is indeed the case.

In the rule of the ε -algorithm, making the change of variable $k = t/\varepsilon^3$ and $n - 1/2 = x/\varepsilon - ct/\varepsilon^3$ and replacing $\varepsilon_k^{(n)}$ by $p + \varepsilon^2 u(x - \varepsilon/2, t)$ where c and p are related by $1 - 2c = 1/p^2$, A. Nagai and J. Satsuma obtained [105]

$$\varepsilon^2 u(x - \varepsilon/2 + c\varepsilon, t + \varepsilon^3) - \varepsilon^2 u(x + \varepsilon/2 - c\varepsilon, t - \varepsilon^3) = \frac{1}{p + \varepsilon^2 u(x + \varepsilon/2, t)} - \frac{1}{p + \varepsilon^2 u(x - \varepsilon/2, t)}.$$

We have, to terms of order ε^5 , the KdV equation

$$u_t - \frac{1}{p^3} uu_x + \frac{1}{48p^2} (1 - p^{-4}) u_{xxx} = 0.$$

Other discrete numerical algorithms, such as the qd , LR , and ρ -algorithms are connected to other discrete or continuous integrable equations (see, for example [112]). Formal orthogonal polynomials, continued fractions, Padé approximation also play a rôle in this topic [113].

By replacing the integer n in the ε -algorithm by a continuous variable, Wynn derived the *confluent form* of the ε -algorithm [149]

$$\varepsilon_{k+1}(t) = \varepsilon_{k-1}(t) + \frac{1}{\varepsilon_k'(t)}$$

with $\varepsilon_{-1}(t) \equiv 0$ and $\varepsilon_0(t) = f(t)$. This algorithm is the continuous counterpart of the ε -algorithm and its aim is to compute $\lim_{t \rightarrow \infty} f(t)$. Setting $N_k(t) = \varepsilon_k'(t)\varepsilon_{k+1}(t)$, A. Nagai, T. Tokihiro and J. Satsuma [106] obtained

$$N_k'(t) = N_k(t)[N_{k-1}(t) - N_{k+1}(t)].$$

The above equation is the Bäcklund transformation of the discrete Toda molecule equation [139].

So, we see that some properties of integrable systems are related to properties of convergence acceleration algorithms. On the other hand, discretizing integrable partial differential equations leads to new sequence transformations which have to be studied from the point of view of their algebraic and acceleration properties. Replacing the second integer k in the confluent form of the ε -algorithm by a continuous variable, Wynn obtained a partial differential equation [152]. Its relation with integrable systems is an open question.

The connection between integrable systems and convergence acceleration algorithms needs to be investigated in more details to fully understand its meaning which is not clear yet.

3. The vector case

In numerical analysis, many iterative methods lead to vector sequences. To accelerate the convergence of such sequences, it is always possible to apply a scalar algorithm componentwise. However, vector sequence transformations, specially built for that purpose, are usually more powerful. The first vector algorithm to be studied was the vector ε -algorithm. It was obtained by Wynn [150] by replacing, in the rule of the scalar ε -algorithm, $1/\Delta\varepsilon_k^{(n)}$ by $(\Delta\varepsilon_k^{(n)})^{-1}$ where the inverse y^{-1} of a vector y is defined by $y^{-1} = y/(y, y)$. Thus, with this definition, the rule of the ε -algorithm can be applied to vector sequences. Using Clifford algebra, J.B. McLeod proved in 1971 [96] that $\forall n, \varepsilon_{2k}^{(n)} = S$ if the sequence (S_n) satisfies $a_0(S_n - S) + \dots + a_k(S_{n+k} - S) = 0$, $\forall n$ with $a_0 a_k \neq 0$, $a_0 + \dots + a_k \neq 0$. This result is only valid for real sequences (S_n) and real a_i 's. Moreover, contrary to the scalar case, this condition is only sufficient. In 1983, Peter R. Graves–Morris [68] extended this result to the complex case using a quite different approach.

A drawback to the development of the theory of the vector ε -algorithm was that it was not known whether a corresponding generalization of Shanks transformation was underlying the algorithm, that is whether the vectors $\varepsilon_k^{(n)}$ obtained by the algorithm could be expressed as ratios of determinants (or some kind of generalization of determinants). This is why Brezinski [17], following the same path as Shanks, tried to construct a vector sequence transformation with the kernel $a_0(S_n - S) + \dots + a_k(S_{n+k} - S) = 0$. He obtained a transformation expressed as a ratio of determinants. He then had to develop a recursive algorithm for avoiding their computation. This was the so-called topological ε -algorithm. This algorithm has many applications, in particular, to the solution of systems of linear equations (it is related to the biconjugate gradient algorithm [18, pp. 185ff]). In the case of a system of nonlinear equations, it gave rise to a generalization of Steffensen's method [13]. That algorithm has a quadratic convergence under some assumptions as established by Hervé Le Ferrand [83] following the ideas presented by Khalide Jbilou and Sadok [75]. The denominator of the vector $\varepsilon_{2k}^{(n)}$ obtained by the vector ε -algorithm was first written as a determinant of dimension $2k + 1$ by Graves–Morris and Chris Jenkins in [69]. The numerator follows immediately by modifying the first row of the denominator, a formula given by Ahmed Salam and Graves–Morris [126]. However, the dimension of the corresponding determinants in the scalar case is only $k + 1$. It was proved by Salam [124] that the vectors $\varepsilon_{2k}^{(n)}$ computed by the vector ε -algorithm can be expressed as a ratio of two *designants* of dimension $k + 1$. A designant is a generalization of a determinant when solving a system of linear equations in a noncommutative algebra. An algebraic approach to this algorithm was given in [125]. This approach, which involves the use of a Clifford algebra, was used in [45] for extending the mechanism given in [41] to the vector and matrix cases. The vector generalization

of the E -algorithm [19] can be explained similarly. This algorithm makes use of a fixed vector y . Jet Wimp [146, pp. 176–177] generalized it using a sequence (y_n) instead of y . Jeannette van Iseghem [140] gave an algorithm for accelerating vector sequences based on the vector orthogonal polynomials she introduced for generalizing Padé approximants to the vector case. Other vector sequence transformations are due to Osada [109] and Jbilou and Sadok [76]. Benchiboun [6] and Abderrahim Messaoudi [100] studied matrix extrapolation algorithms.

We have seen that, in the scalar case, the kernels of sequence transformations may be expressed as relationships with constant coefficients. This is also the case for the vector and the topological ε -algorithms and the vector E -algorithm. The first (and, to my knowledge, only) transformation treating a relationship with varying coefficients was introduced in [42]. The theory developed there also explains why the case of a relationship with non-constant coefficients is a difficult problem in the scalar case and why it could be solved, on the contrary, in the vector case. The reason is that the number of unknown coefficients appearing in the expression of the kernel must be strictly less than the dimension of the vectors. Brezinski in [34] proposed a general methodology for constructing vector sequence transformations. It leads to a unified presentation of several approaches to the subject and to new results. He also discussed applications to linear systems. In fact, as showed by Sidi [133], and Jbilou and Sadok [75], vector sequence transformations are closely related to projection methods for the solution of systems of equations. In particular, the RPA, a vector sequence transformation defined by Brezinski [20] was extensively studied by Messaoudi who showed its connections to direct and iterative methods for solving systems of linear equations [98,99].

Vector sequence transformations lead to new methods for the solution of systems of nonlinear equations. They also have other applications. First of all, it is quite important to accelerate the convergence of iterative methods for the solution of systems of linear equations, see [32,33,36]. Special vector extrapolation techniques were designed for the regularization of ill-posed linear systems in [43] and the idea of extrapolation was used in [35] to obtain estimates of the norm of the error when solving a system of linear equations by an arbitrary method, direct or iterative.

General theoretical results similar to those obtained in the scalar case are still lacking in the vector case although some partial results have been obtained. Relevant results on quasilinear transformations are in the papers by Sadok [123] and Benazzouz [8]. The present author proposed a mechanism for vector sequence transformations in [45,34].

4. Conclusions and perspectives

In this paper, I have tried to give a survey of the development of convergence acceleration methods for scalar and vector sequences in the 20th century. These methods are based on the idea of extrapolation. Since a universal algorithm for accelerating the convergence of all sequences cannot exist (and this is even true for some restricted classes of sequences), it was necessary to define and study a large variety of algorithms, each of them being appropriate for some special subsets of sequences.

It is, of course, always possible to construct other convergence acceleration methods for scalar sequences. However, to be of interest, such new processes must provide a major improvement over existing ones. For scalar sequence transformations, the emphasis must be placed on the theory rather than on special devices (unless a quite powerful one is found) and on the application of new

methods to particular algorithms in numerical analysis and to various domains of applied sciences. In particular, the connection between convergence acceleration algorithms and continuous and discrete integrable systems brings a different and fresh look to both domains and could be of benefit to them.

An important problem in numerical analysis is the solution of large, sparse systems of linear equations. Most of the methods used nowadays are projection methods. Often the iterates obtained in such problems must be subject to acceleration techniques. However, many of the known vector convergence acceleration algorithms require the storage of too many vectors to be useful. New and cheaper acceleration algorithms are required. This difficult project, in my opinion, offers many opportunities for future research.

In this paper, I only briefly mentioned the confluent algorithms whose aim is the computation of the limit of a function when the variable tends to infinity (the continuous analog of the problem of convergence acceleration for a sequence). This subject and its applications will provide fertile ground for new discoveries.

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On the history of multivariate polynomial interpolation

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Abstract

Multivariate polynomial interpolation is a basic and fundamental subject in Approximation Theory and Numerical Analysis, which has received and continues receiving not deep but constant attention. In this short survey, we review its development in the first 75 years of this century, including a pioneering paper by Kronecker in the 19th century. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

Interpolation, by polynomials or other functions, is a rather old method in applied mathematics. This is already indicated by the fact that, apparently, the word “interpolation” itself has been introduced by J. Wallis as early as 1655 as it is claimed in [13]. Compared to this, polynomial interpolation in *several variables* is a relatively new topic and probably only started in the second-half of the last century with work in [6,22]. If one considers, for example, the *Encyklopädie der Mathematischen Wissenschaften* [13] (Encyclopedia of Math. Sciences), originated by the *Preußische Akademie der Wissenschaften* (Prussian Academy of Sciences) to sum up the “state of art” of mathematics at its time, then the part on interpolation, written by J. Bauschinger (Bd. I, Teil 2), mentions only one type of multivariate interpolation, namely (tensor) products of sine and cosine functions in two variables, however, without being very specific. The French counterpart, the *Encyclopédie de Sciences Mathématiques* [14], also contains a section on interpolation (Tome I, vol. 4), where Andoyer translated and extended Bauschinger’s exposition. Andoyer is even more

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explicit with his opinion on multivariate polynomial interpolation, by making the following statement which we think that time has contradicted:

Il est manifeste que l'interpolation des fonctions de plusieurs variables ne demande aucun principe nouveau, car dans tout ce qui précède le fait que la variable indépendante était unique n'a souvent joué aucun rôle.¹

Nevertheless, despite of Andoyer's negative assessment, multivariate polynomial interpolation has received not deep but constant attention from one part of the mathematical community and is today a basic subject in Approximation Theory and Numerical Analysis with applications to many mathematical problems. Of course, this field has definitely been influenced by the availability of computational facilities, and this is one of the reasons that more papers have been published about this subject in the last 25 years than in the preceding 75 ones.

To our knowledge, there is not any paper before the present one surveying the early papers and books on multivariate polynomial interpolation. Our aim is a first, modest attempt to cover this gap. We do not claim to be exhaustive and, in particular, recognize our limitations with respect to the Russian literature. Moreover, it has to be mentioned that the early results on multivariate interpolation usually appear in the context of many different subjects. For example, papers on cubature formulas frequently have some part devoted to it. Another connection is Algebraic Geometry, since the solvability of a multivariate interpolation problem relies on the fact that the interpolation points do not lie on an algebraic surface of a certain type. So it is difficult to verify precisely if and when a result appeared somewhere for the first time or if it had already appeared, probably even in an implicit way, in a different context. We remark that another paper in this volume [25] deals, complementarily, with recent results in the subject, see also [16].

Along the present paper we denote by Π_k^d the space of d -variate polynomials of total degree not greater than k .

2. Kronecker, Jacobi and multivariate interpolation

Bivariate interpolation by the tensor product of univariate interpolation functions, that is when the variables are treated separately, is the classical approach to multivariate interpolation. However, when the set of interpolation points is not a Cartesian product grid, it is impossible to use that idea. Today, given any set of interpolation points, there exist many methods² to construct an adequate polynomial space which guarantees unisolvence of the interpolation problem. Surprisingly, this idea of constructing an appropriate interpolation space was already pursued by Kronecker [22] in a widely unknown paper from 1865, which seems to be the first treatment of multivariate polynomial interpolation with respect to fairly arbitrary point configurations. Besides the mathematical elegance of this approach, we think it is worthwhile to devote some detailed attention to this paper and to resolve its main ideas in today's terminology, in particular, as it uses the "modern" approach of connecting polynomial interpolation to the theory of polynomial ideals.

¹ It is clear that the interpolation of functions of several variables does not demand any new principles because in the above exposition the fact that the variable was unique has not played frequently any role.

² See [16,25] for exposition and references.

Kronecker’s method to construct an interpolating polynomial assumes that the disjoint nodes $z_1, \dots, z_N \in \mathbb{C}^d$ are given in *implicit* form, i.e., they are (all) the common *simple* zeros of d polynomials $f_1, \dots, f_d \in \mathbb{C}[z] = \mathbb{C}[\zeta_1, \dots, \zeta_d]$. Note that the nonlinear system of equations

$$f_j(\zeta_1, \dots, \zeta_d) = 0, \quad j = 1, \dots, d, \tag{1}$$

is a *square* one, that is, the number of equations and the number of variables coincide. We are interested in the *finite* variety V of solutions of (1) which is given as

$$V := \{z_1, \dots, z_N\} = \{z \in \mathbb{C}^d : f_1(z) = \dots = f_d(z) = 0\}. \tag{2}$$

The *primary decomposition* according to the variety V allows us to write the ideal $\mathcal{I}(V) = \{p : p(z) = 0, z \in V\}$ as

$$\mathcal{I}(V) = \bigcap_{k=1}^N \langle \zeta_1 - \zeta_{k,1}, \dots, \zeta_d - \zeta_{k,d} \rangle,$$

where $z_k = (\zeta_{k,1}, \dots, \zeta_{k,d})$. In other words, since $f_k \in \mathcal{I}(V)$, $k = 1, \dots, d$, any of the polynomials f_1, \dots, f_d can be written, for $k = 1, \dots, N$, as

$$f_j = \sum_{i=1}^d g_{i,j}^k(\cdot) (\zeta_i - \zeta_{k,i}), \tag{3}$$

where $g_{i,j}^k$ are appropriate polynomials. Now consider the $d \times d$ square matrices of polynomials

$$G_k = [g_{i,j}^k : i, j = 1, \dots, d], \quad k = 1, \dots, N$$

and note that, due to (3), and the assumption that $f_j(z_k) = 0$, $j = 1, \dots, d$, $k = 1, \dots, N$, we have

$$0 = \begin{bmatrix} f_1(z_j) \\ \vdots \\ f_d(z_j) \end{bmatrix} = G_k(z_j) \begin{bmatrix} (\zeta_{j,1} - \zeta_{k,1}) \\ \vdots \\ (\zeta_{j,d} - \zeta_{k,d}) \end{bmatrix}, \quad k = 1, \dots, N. \tag{4}$$

Since the interpolation nodes are assumed to be *disjoint*, this means that for all $j \neq k$ the matrix $G_k(z_j)$ is *singular*, hence the determinant of $G_k(z_j)$ has to be zero. Moreover, the assumption that z_1, \dots, z_N are *simple* zeros guarantees that $\det G_k(z_k) \neq 0$. Then, Kronecker’s interpolant takes, for any $f : \mathbb{C}^d \rightarrow \mathbb{C}$, the form

$$Kf = \sum_{j=1}^N f(z_j) \frac{\det G_k(\cdot)}{\det G_k(z_k)}. \tag{5}$$

Hence,

$$\mathcal{P} = \text{span} \left\{ \frac{\det G_k(\cdot)}{\det G_k(z_k)} : k = 1, \dots, N \right\}$$

is an interpolation space for the interpolation nodes z_1, \dots, z_N . Note that this method does not give only *one* interpolation polynomial but in general *several different* interpolation spaces, depending on how the representation in (3) is chosen. In any way, note that for each polynomial $f \in \mathbb{C}[z]$ the difference

$$f - \sum_{j=1}^N f(z_j) \frac{\det G_k(z)}{\det G_k(z_k)}$$

belongs to the ideal $\langle f_1, \dots, f_d \rangle$, hence there exist polynomials q_1, \dots, q_d such that

$$f - \sum_{j=1}^N f(z_j) \frac{\det G_k(z)}{\det G_k(z_k)} = \sum_{j=1}^d q_j f_j. \tag{6}$$

Moreover, as Kronecker points out, the “magic” polynomials $g_{i,j}^k$ can be chosen such that their leading homogeneous terms, say $G_{i,j}^k$, coincide with the leading homogeneous terms of $(1/\deg f_j)\partial f_j/\partial \zeta_i$. If we denote by F_j the leading homogeneous term of f_j , $j = 1, \dots, d$, then this means that

$$G_{i,j}^k = \frac{1}{\deg F_j} \frac{\partial F_j}{\partial \zeta_i}, \quad i, j = 1, \dots, d, \quad k = 1, \dots, N. \tag{7}$$

But this implies that the homogeneous leading term of the “fundamental” polynomials $\det G_k$ coincides, after this particular choice of $g_{i,j}^k$, with

$$g = \frac{1}{\deg f_1 \cdots \deg f_d} \det \left[\frac{\partial F_j}{\partial \zeta_i} : i, j = 1, \dots, d \right],$$

which is independent of k now; in other words, there exist polynomials \hat{g}_k , $k = 1, \dots, N$, such that $\deg \hat{g}_k < \deg g$ and $\det G_k = g + \hat{g}_k$. Moreover, g is a homogeneous polynomial of degree at most $\deg f_1 + \dots + \deg f_d - d$. Now, let p be any polynomial, then

$$Kp = \sum_{j=1}^N p(z_j) \frac{\det G_j(\cdot)}{\det G_j(z_j)} = g \sum_{j=1}^N \frac{p(z_j)}{\det G_j(z_j)} + \sum_{j=1}^N \frac{p(z_j)}{\det G_j(z_j)} \hat{g}_j. \tag{8}$$

Combining (8) with (6) then yields the existence of polynomials q_1, \dots, q_d such that

$$p = g \sum_{j=1}^N \frac{p(z_j)}{\det G_j(z_j)} + \sum_{j=1}^N \frac{p(z_j)}{\det G_j(z_j)} \hat{g}_j + \sum_{j=1}^d q_j f_j$$

and comparing homogeneous terms of degree $\deg g$ Kronecker realized that either, for any p such that $\deg p < \deg g$,

$$\sum_{j=1}^N \frac{p(z_j)}{\det G_j(z_j)} = 0 \tag{9}$$

or there exist homogeneous polynomials h_1, \dots, h_d such that

$$g = \sum_{j=1}^d h_j \det F_j. \tag{10}$$

The latter case, Eq. (10), says (in algebraic terminology) that there is a *syzygy* among the leading terms of the polynomials F_j , $j = 1, \dots, d$, and is equivalent to the fact that $N < \deg f_1 \cdots \deg f_d$, while (9) describes and even characterizes the *complete intersection case* that $N = \deg f_1 \cdots \deg f_d$. In his paper, Kronecker also mentions that the condition (10) has been overlooked in [21]. Jacobi dealt there with the common zeros of two bivariate polynomials and derived *explicit* representations for the functional

$$[z_1, \dots, z_N]f := \sum_{j=1}^N \frac{f(z_j)}{\det G_j(z_j)}, \tag{11}$$

which behaves very much like a divided difference, since it is a combination of point evaluations which, provided that (9) hold true, annihilates $\Pi_{\deg g-1}^d$.

In addition, Kronecker refers to a paper [6] which he says treats the case of symmetric functions, probably elementary symmetric polynomials. Unfortunately, this paper is unavailable to us so far.

3. Bivariate tables, the natural approach

Only very few research papers on multivariate polynomial interpolation were published during the first part of this century. In the classical book *Interpolation* [45], where one section (Section 19) is devoted to this topic, the author only refers to two related papers, recent at that time (1927), namely [27,28]. The latter one [28], turned out to be inaccessible to us, unfortunately, but it is not difficult to guess that it might have pursued a tensor product approach, because this is the unique point of view of [45] (see also [31]).

The formulas given in [27] are Newton formulas for tensor product interpolation in two variables, and the author, Narumi, claims (correctly) that they can be extended to “many variables”. Since it is a tensor product approach, the interpolation points are of the form (x_i, y_j) , $0 \leq i \leq m$, $0 \leq j \leq n$, with x_i, y_j arbitrarily distributed on the axes OX and OY , respectively. Bivariate divided differences for these sets of points are obtained in [27], by recurrence, separately for each variable. With the usual notations, the interpolation formula from [27] reads as

$$p(x, y) = \sum_{i=0}^m \sum_{j=0}^n f[x_0, \dots, x_i; y_0, \dots, y_j] \prod_{h=0}^{i-1} (x - x_h) \prod_{k=0}^{j-1} (y - x_k), \tag{12}$$

where empty products have the value 1. Remainder formulas based on the mean value theorem are also derived recursively from the corresponding univariate error formulas in [27]. For f sufficiently smooth there exist values ξ, ξ', η, η' such that

$$R(x, y) = \frac{\partial^{m+1} f(\xi, y) \prod_{h=0}^m (x - x_h)}{\partial x^{m+1} (m+1)!} + \frac{\partial^{n+1} f(x, \eta) \prod_{k=0}^n (y - y_k)}{\partial y^{n+1} (n+1)!} - \frac{\partial^{m+n+2} f(\xi', \eta') \prod_{h=0}^m (x - x_h) \prod_{k=0}^n (y - y_k)}{\partial x^{m+1} \partial y^{n+1} (m+1)! (n+1)!}. \tag{13}$$

The special case of equidistant points on both axes is particularly considered in [27], and since the most popular formulas at that time were based on finite differences with equally spaced arguments, Narumi shows how to extend Gauss, Bessel and Stirling univariate interpolation formulas for equidistant points to the bivariate case by tensor product. He also applies the formulas he obtained to approximate the values of bivariate functions, but he also mentions that some of his formulas had been already used in [49].

In [45], the Newton formula (12) is obtained in the same way, with the corresponding remainder formula (13). Moreover, Steffensen considers a more general case, namely when for each i , $0 \leq i \leq m$, the interpolation points are of the form y_0, \dots, y_{n_i} , with $0 \leq n_i \leq n$. Now with a similar argument the interpolating polynomial becomes

$$p(x, y) = \sum_{i=0}^m \sum_{j=0}^{n_i} f[x_0, \dots, x_i; y_0, \dots, y_j] \prod_{h=0}^{i-1} (x - x_h) \prod_{k=0}^{j-1} (y - x_k) \tag{14}$$

with a slightly more complicated remainder formula. The most interesting particular cases occur when $n_i = n$, which is the Cartesian product considered above, and when $n_i = m - i$. This *triangular* case (triangular not because of the geometrical distribution of the interpolation points, but of the indices (i, j)), gives rise to the interpolating polynomial

$$p(x, y) = \sum_{i=0}^m \sum_{j=0}^{m-i} f[x_0, \dots, x_i; y_0, \dots, y_j] \prod_{h=0}^{i-1} (x - x_h) \prod_{k=0}^{j-1} (y - x_k), \quad (15)$$

that is

$$p(x, y) = \sum_{0 \leq i+j \leq m} f[x_0, \dots, x_i; y_0, \dots, y_j] \prod_{h=0}^{i-1} (x - x_h) \prod_{k=0}^{j-1} (y - x_k). \quad (16)$$

Steffensen refers for this formula to Biermann's lecture notes [4] from 1905, and actually it seems that Biermann has been the first who considered polynomial interpolation on the triangular grid in a paper [3] from 1903 (cf. [44]) in the context of cubature.

Since the triangular case corresponds to looking at the “lower triangle” of the tensor product situation only, this case can be resolved by tensor product methods. In particular, the respective error formula can be written as

$$R(x, y) = \sum_{i=0}^{m+1} \frac{\partial^{m+1} f(\xi_i, \eta_i)}{\partial x^i \partial y^{m+1-i}} \frac{\prod_{h=0}^{i-1} (x - x_h)}{i!} \frac{\prod_{k=0}^{m-i} (y - y_k)}{(m - i + 1)!}. \quad (17)$$

In the case of Cartesian product Steffensen also provides the Lagrange formula for (12), which can be obviously obtained by tensor product of univariate formulas.

Remainder formulas based on intermediate points (ξ_i, η_i) can be written in many different forms. For them we refer to Stancu's paper [44] which also contains a brief historical introduction where the author refers, among others, to [3,15,27,40,41]. Multivariate remainder formulas with Peano (spline) kernel representation, however, have not been derived until very recently in [42] and, in particular, in [43] which treats the triangular situation.

4. Salzer's papers: from bivariate tables to general sets

In 1944, Salzer [33] considered the interpolation problem at points of the form $(x_1 + s_1 h_1, \dots, x_n + s_n h_n)$ where

- (i) (x_1, \dots, x_n) is a given point in \mathbb{R}^n ,
- (ii) h_1, \dots, h_n are given real numbers,
- (iii) s_1, \dots, s_n are nonnegative integers summing up to m .

This is the multivariate extension of the triangular case (16) for equally spaced arguments, where finite differences can be used. Often, different names are used for the classical Newton interpolation formula in the case of equally spaced arguments using forward differences: Newton–Gregory, Harriot–Briggs, also known by Mercator and Leibnitz, etc. See [18] for a nice discussion of this issue. In [33], Salzer takes the natural multivariate extension of this formula considering the polynomial $q(t_1, \dots, t_n) := p(x_1 + t_1 h_1, \dots, x_n + t_n h_n)$ of total degree not greater than m in the variables t_1, \dots, t_n , which interpolates a function $f(x_1 + t_1 h_1, \dots, x_n + t_n h_n)$ at the points corresponding to $t_i = s_i$, $i = 1, \dots, n$,

where the s_i are all nonnegative integers such that $0 \leq s_1 + \dots + s_n \leq m$. The formula, which is called in [33] a *multiple Gregory–Newton formula*, is rewritten there in terms of the values of the function f at the interpolation points, i.e., in the form

$$q(t_1, \dots, t_n) = \sum_{s_1 + \dots + s_n \leq m} \binom{t_1}{s_1} \cdots \binom{t_n}{s_n} \binom{m - t_1 - \dots - t_n}{m - s_1 - \dots - s_n} f(x_1 + s_1 h_1, \dots, x_n + s_n h_n). \quad (18)$$

Note that (18) is the Lagrange formula for this interpolation problem. Indeed, each function

$$\binom{t_1}{s_1} \cdots \binom{t_n}{s_n} \binom{m - t_1 - \dots - t_n}{m - s_1 - \dots - s_n} \quad (19)$$

is a polynomial in t_1, \dots, t_n of total degree m which vanishes at all points (t_1, \dots, t_n) with t_i nonnegative integers $0 \leq t_1 + \dots + t_n \leq m$, except at the point (s_1, \dots, s_n) , where it takes the value 1. In particular, for $n = 1$ we get the well-known univariate Lagrange polynomials

$$\ell_s(t) = \binom{t}{s} \binom{m - t}{m - s} = \prod_{\substack{0 \leq i \leq m, \\ i \neq s}} \frac{t - i}{s - i}$$

for $s = 0, \dots, m$.

Salzer used these results in [34] to compute tables for the polynomials (18) and, some years later in [35], he studied in a similar form how to get the Lagrange formula for the more general case of formula (16), even starting with this formula. He obtained the multivariate Lagrange polynomials by a rather complicated expression involving the univariate ones.

It should be noted that several books related to computations and numerical methods published around this time include parts on multivariate interpolation to some extent, surprisingly, more than most of the recent textbooks in Numerical Analysis. We have already mentioned Steffensen’s book [45], but we should also mention Whittaker and Robinson [51, pp. 371–374], Mikeladze [26, Chapter XVII] and especially Kunz [23, pp. 248–274], but also Isaacson and Keller [20, pp. 294–299] and Berezin and Zhidkov [2, pp. 156–194], although in any of them not really much more than in [45] is told.

In [36,37], Salzer introduced a concept of bivariate divided differences abandoning the idea of iteration for each variable x and y taken separately. Apparently, this was the first time (in spite of the similarity with (11)), that bivariate divided differences were explicitly defined for irregularly distributed sets of points. Divided differences with repeated arguments are also considered in [37] by coalescence of the ones with different arguments. Since [36] was just a first attempt of [37], we only explain the latter one. Salzer considers the set of monomials $\{x^i y^j\}$, with i, j nonnegative integers, ordered in a graded lexical term order, that is,

$$(i, j) < (h, k) \Leftrightarrow i + j < h + k \quad \text{or} \quad i + j = h + k, i > h. \quad (20)$$

Hence, the monomials are listed as

$$\{1, x, y, x^2, xy, y^2, x^3, \dots\}. \quad (21)$$

For any set of $n + 1$ points (x_i, y_i) , Salzer defines the associated divided difference

$$[01 \dots n]f := \sum_{k=0}^n A_k f(x_k, y_k), \quad (22)$$

choosing the coefficients A_k in such a form that (22) vanishes when f is any of the first n monomials of list (21) and takes the value 1 when f is the $(n + 1)$ st monomial of that list. In other words, the coefficients A_k are the solution of the linear system

$$\begin{aligned} \sum_{k=0}^n A_k x_k^i y_k^j &= 0, & x^i y^j \text{ any of the first } n \text{ monomials of (21),} \\ \sum_{k=0}^n A_k x_k^i y_k^j &= 1, & x^i y^j \text{ the } (n + 1)\text{th monomial of (21).} \end{aligned} \quad (23)$$

These generalized divided differences share some of the properties of the univariate ones but not all. Moreover, they have some limitations, for example, they exist only if the determinant of the coefficients in (23) is different from zero, and one has no control of that property in advance. On the other hand, observe that for example the simple divided difference with two arguments (x_0, y_0) and (x, y) , which is

$$\frac{f(x, y) - f(x_0, y_0)}{x - x_0},$$

gives, when applied to $f(x, y) = xy$, the rational function

$$\frac{xy - x_0 y_0}{x - x_0}$$

and not a polynomial of lower degree. In fact, Salzer's divided differences did not have great success. Several other definitions of multivariate divided differences had appeared since then, trying to keep as many as possible of the good properties of univariate divided differences, cf. [16].

5. Reduction of a problem to other simpler ones

Around the 1950s an important change of paradigm happened in multivariate polynomial interpolation, as several people began to investigate more general distributions of points, and not only (special) subsets of Cartesian products. So, when studying cubature formulae [32], Radon observed the following in 1948: if a bivariate interpolation problem with respect to a set $T \subset \mathbb{R}^2$ of $\binom{k+2}{2}$ interpolation points is unisolvent in Π_k^2 , and U is a set of $k + 2$ points on an arbitrary straight line $\ell \subset \mathbb{R}^2$ such that $\ell \cap T = \emptyset$, then the interpolation problem with respect to $T \cup U$ is unisolvent in Π_{k+1}^2 . Radon made use of this observation to build up point sets which give rise to unisolvent interpolation problems for Π_m recursively by degree. Clearly, these interpolation points immediately yield interpolatory cubature formulae.

The well-known Bézout theorem, cf. [50], states that two planar algebraic curves of degree m and n , with no common component, intersect each other at exactly mn points in an algebraic closure of the underlying field, counting multiplicities. This theorem has many interesting consequences for bivariate interpolation problems, extensible to higher dimensions. For example, no unisolvent interpolation problem in Π_n^2 can have more than $n + 1$ collinear points. Radon's method in [32] is a consequence of this type of observations, and some other more recent results of different authors can also be deduced in a similar form, as we shall see later.

Another example of a result which shows the more general point of view taken in multivariate interpolation at that time is due to Thacher Jr. and Milne [47] (see also [48]). Consider two univariate interpolation problems in Π_{n-1}^1 , with T_1, T_2 as respective sets of interpolation points, both of cardinality n . Assume that $T_1 \cap T_2$ has cardinality $n - 1$, hence $T = T_1 \cup T_2$ has cardinality $n + 1$. The univariate Aitken–Neville interpolation formula combines the solutions of the two smaller problems based on T_1 and T_2 to obtain the solution in Π_n^1 of the interpolation problem with T as the underlying set of interpolation points. The main idea is to find a *partition of unity*, in this case affine polynomials ℓ_1, ℓ_2 , i.e., $\ell_1 + \ell_2 = 1$, such that

$$\ell_1(T_2 \setminus T_1) = \ell_2(T_1 \setminus T_2) = 0$$

and then combine the solutions p_1, p_2 with respect to T_1, T_2 , into the solution $\ell_1 p_1 + \ell_2 p_2$ with respect to T . This method was developed in the 1930s independently by Aitken and Neville with the goal to avoid the explicit use of divided differences in the computation of univariate Lagrange polynomial interpolants.

It was exactly this idea which Thatcher and Milne extended to the multivariate case in [47]. Let us sketch their approach in the bivariate case. For example, consider an interpolation problem with 10 interpolation points, namely, the set $T = \{(i, j) : 0 \leq i + j \leq 3\}$, where i, j are nonnegative integers, and the interpolation space Π_3^2 . The solution p_T of this problem is obtained in [47] from the solutions $p_{T_k} \in \Pi_2^2$, $k = 1, 2, 3$, of the 3 interpolation problems with respect to the six-point sets $T_k \subset T$, $k = 1, 2, 3$, where

$$T_1 = \{(i, j) : 0 \leq i + j \leq 2\},$$

$$T_2 = \{(i, j) : (i, j) \in T, i > 0\},$$

$$T_3 = \{(i, j) : (i, j) \in T, j > 0\}.$$

Then,

$$p_T = \ell_1 p_{T_1} + \ell_2 p_{T_2} + \ell_3 p_{T_3},$$

where ℓ_k , $k = 1, 2, 3$ are appropriate polynomials of degree 1. In fact, in this case these polynomials are the barycentric coordinates relative to the simplex $(0, 0), (3, 0), (0, 3)$ and thus a partition of unity. In [47] the problem is studied in d variables and in that case $d + 1$ “small” problems, with respective interpolation sets T_k , $k = 1, \dots, d$, with a simplicial structure (the analogue of the triangular grid), are used to obtain the solution of the full problem with $T = T_1 \cap \dots \cap T_{d+1}$ as interpolation points.

In 1970, Guenter and Roetman [19], among other observations, made a very interesting remark, which connects to the Radon/Bézout context and deserves to be explained here. Let us consider a set T of $\binom{m+d}{d}$ points in \mathbb{R}^d , where exactly $\binom{m+d-1}{d-1}$ of these points lie on a hyperplane H . Then $T \setminus H$ consists of $\binom{m-1+d}{d}$ points. Let us denote by $\Pi_{d,H}^m$ the space of polynomials of Π_d^m with the variables restricted to H , which is isomorphic to Π_{d-1}^m . If the interpolation problems defined by the sets $T \setminus H$ and $T \cap H$ are unisolvent in the spaces Π_d^{m-1} and $\Pi_{d,H}^m$, respectively, then the interpolation problem defined by T is unisolvent in Π_d^m . In other words, the idea is to decompose, whenever possible, a problem of degree m and d variables into two simpler problems, one of degree m and $d - 1$ variables and the other one with degree $m - 1$ and d variables.

6. The finite element approach

In 1943, Courant [11] suggested a finite difference method applicable to boundary value problems arising from variational problems. It is considered one of the motivations of the finite element method, which emerged from the engineering literature along the 1950s. It is a variational method of approximation which makes use of the Rayleigh–Ritz–Galerkin technique. The method became very successful, with hundreds of technical papers published (see, e.g., the monograph [52]), even before its mathematical basis was completely understood at the end of the 1960s.

Involved in the process of the finite element method there are local polynomial interpolation problems, generally for polynomials of low degree, thus, with only few interpolation data. The global solution obtained by solving all the local interpolation problems is a piecewise polynomial of a certain regularity, depending on the amount and type of interpolation data in the common boundary between pieces. Some of the interest in multivariate polynomial interpolation along the 1960/1970s was due to this method. Among the most interesting mathematical papers of that time in Finite Elements, we can mention [53,5], see also the book [46] by Strang and Fix, but, in our opinion, the most relevant papers and book from the point of view of multivariate polynomial interpolation are due to Ciarlet et al., for example [7–9].

In 1972, Nicolaidis [29,30] put the classical problem of interpolation on a simplicial grid of $\binom{m+d}{d}$ points of \mathbb{R}^d , regularly distributed, forming what he called a *principal lattice*, into the finite element context. He actually used barycentric coordinates for the Lagrange formula, and moreover gave the corresponding error representations, see also [7]. However, much of this material can already be found in [3]. In general, taking into account that these results appeared under different titles, in a different context and in journals not accessible everywhere, it is not so surprising any more, how often the basic facts on the interpolation problem with respect to the simplicial grid had been rediscovered.

7. Hermite problems

The use of partial or directional derivatives as interpolation data in the multivariate case had not received much attention prior to the finite element method, where they were frequently used. It seems natural to approach partial derivatives by coalescence, as in univariate Hermite interpolation problems. However, things are unfortunately much more complicated in several variables. As it was already pointed out by Salzer and Kimbro [39] in 1958, the Hermite interpolation problem based on the values of a bivariate function $f(x, y)$ at two distinct points $(x_1, y_1), (x_2, y_2)$ and on the values of the partial derivatives $\partial f/\partial x, \partial f/\partial y$ at each of these two points is not solvable in the space Π_2^2 for any choice of points, although the number of interpolation conditions coincides with the dimension of the desired interpolation space. Some years later, Ahlin [1] circumvented some of these problems by using a tensor product approach: k^2 derivatives $\partial^{p+q} f/\partial x^p \partial y^q$ with $0 \leq p, q \leq k-1$ are prescribed at the n^2 points of a Cartesian product. The interpolation space is the one spanned by $x^\alpha y^\beta$ with $0 \leq \alpha, \beta \leq nk-1$ and a formula for the solution is easily obtained.

We must mention that Salzer came back to bivariate interpolation problems with derivatives in [38] studying *hyperosculatory interpolation* over Cartesian grids, that is, interpolation problems where all partial derivatives of first and second order and the value of the function are known at the

interpolation points. Salzer gave some special configurations of points which yield solvability of this type of interpolation problem in an appropriate polynomial space and also provided the corresponding remainder formulae.

Nowadays, Hermite and Hermite–Birkhoff interpolation problems have been studied much more systematically, see [16,25] for references.

8. Other approaches

In 1966, Coatmelec [10] studied the approximation of functions of several variables by linear operators, including interpolation operators. At the beginning of the paper, he only considered interpolation operators based on values of point evaluations of the function, but later he also used values of derivatives. In this framework he obtained some qualitative and quantitative results on the approximation order of polynomial interpolation. At the end of [10], Coatmelec also includes some examples in \mathbb{R}^2 of points which are distributed irregularly along lines: $n + 1$ of the points on a line r_0 , n of them on another line r_1 , but not on r_0 , and so on until 1 point is chosen on a line r_n but not on $r_0 \cup \dots \cup r_{n-1}$. He then points out the unsolvability of the corresponding interpolation problem in Π_n^2 which is, in fact, again a consequence of Bézout’s theorem as in [32].

In 1971, Glaeser [17] considers Lagrange interpolation in several variables from an abstract algebraic/analytic point of view and acknowledges the inconvenience of working with particular systems of interpolation points due to the possibility of the nonexistence of a solution, in contrast to the univariate case. This is due to the nonexistence of polynomial spaces of dimension $k > 1$ in more than one variable such that the Lagrange interpolation problem has a unique solution for any system of k interpolation points. In other words, there are no nontrivial Haar (or Chebyshev) spaces any more for two and more variables, cf. [12] or [24]. In [17], polynomial spaces with dimension greater than the number of interpolation conditions are considered in order to overcome this problem. Glaeser investigated these *underdetermined* systems which he introduced as *interpolation schemes* in [17] and also studied the problem of how to particularize the affine space of all solutions of a given interpolation problem in order to obtain a unique solution. This selection process is done in such a way that it controls the variation of the solution when two systems of interpolation points are very “close” to each other, with the goal to obtain a continuous selection process.

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Elimination techniques: from extrapolation to totally positive matrices and CAGD

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Abstract

In this survey, we will show some connections between several mathematical problems such as extrapolation, linear systems, totally positive matrices and computer-aided geometric design, with elimination techniques as the common tool to deal with all of them. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

Matrix elimination techniques are basic tools in many mathematical problems. In this paper we will show their crucial role in some results that various authors with us have obtained in two problems apparently distant: extrapolation and computer-aided geometric design (CAGD). A brief overview of how things were developed over time will show that, once again, two results which are apparently far from each other, even obtained by different groups in different countries, are the natural consequence of a sequence of intermediate results.

Newton's interpolation formula is a classical tool for constructing an interpolating polynomial by recurrence, by using divided differences. In the 1930s, Aitken [1] and Neville [52] derived independently of each other algorithms to compute the interpolating polynomial from the solutions of two simpler interpolation problems, avoiding the explicit use of divided differences. Some papers, [38,46] among others, extended both approaches at the beginning of the 1970s, to the more general setting of Chebyshev systems. Almost simultaneously, extrapolation methods were being studied and extended by several authors, as Schneider [54], Brezinski [4,5,7], Håvie [31–33], Mühlbach [39–42,48] and Gasca and López-Carmona [19]. For a historical overview of extrapolation methods confer Brezinski's contribution [6] to this volume and the book [8]. It must be remarked that the

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techniques used by these authors were different, and that frequently the results obtained using one of these techniques induced some progress in the other ones, in a very cooperative form.

However, it is clear that the basic role in all these papers was played by elimination techniques. In [21] we studied general elimination strategies, where one strategy which we called Neville elimination proved to be well suited to work with some special classes of matrices, in particular *totally positive matrices* (that are matrices with all subdeterminants nonnegative).

This was the origin of a series of papers [24–27] where the properties of Neville elimination were carefully studied and its application to totally positive matrices allowed a much better knowledge of these matrices. Since one of the applications of totally positive matrices is CAGD, the results obtained for them have given rise in the last years to several other papers as [28,11,12]. In [11,12] Carnicer and Peña proved the optimality in their respective spaces of some well-known function bases as Bernstein polynomials and B-splines in the context of shape preserving representations. Neville elimination has appeared, once again, as a way to construct other bases with similar properties.

2. Extrapolation and Schur complement

A k -tuple $L = (\ell_1, \dots, \ell_k)$ of natural numbers, with $\ell_1 < \dots < \ell_k$, will be called an *index list of length k* over \mathbb{N} . For $I = (i_1, \dots, i_m)$ and $J = (j_1, \dots, j_n)$ two index lists over \mathbb{N} , we write $I \subset J$ iff every element of I is an element of J . Generally, we shall use for index lists the same notations as for sets emphasizing that $I \setminus J, I \cap J, I \cup J \dots$ always have to be ordered as above.

Let $A = (a_{ij}^i)$ be a real matrix and $I = (i_1, \dots, i_m)$ and $J = (j_1, \dots, j_n)$ index lists contained, respectively, in the index lists of rows and columns of A . By

$$A \begin{pmatrix} J \\ I \end{pmatrix} = A \begin{pmatrix} j_1, \dots, j_n \\ i_1, \dots, i_m \end{pmatrix} = (a_{i_\mu}^{j_\nu})_{\mu=1, \dots, m}^{\nu=1, \dots, n} \in \mathbb{R}^{m \times n},$$

we denote the *submatrix* of A with list of rows I and list of columns J .

If $I^\circ, I^{\circ'}$ and $J^\circ, J^{\circ'}$ are partitions of I and J , respectively, i.e., $I^\circ \cup I^{\circ'} = I, I^\circ \cap I^{\circ'} = \emptyset, J^\circ \cup J^{\circ'} = J, J^\circ \cap J^{\circ'} = \emptyset$, we represent $A \begin{pmatrix} J \\ I \end{pmatrix}$ in a corresponding partition

$$A \begin{pmatrix} J \\ I \end{pmatrix} = \begin{pmatrix} A \begin{pmatrix} J^\circ \\ I^\circ \end{pmatrix} & A \begin{pmatrix} J^{\circ'} \\ I^\circ \end{pmatrix} \\ A \begin{pmatrix} J^\circ \\ I^{\circ'} \end{pmatrix} & A \begin{pmatrix} J^{\circ'} \\ I^{\circ'} \end{pmatrix} \end{pmatrix}. \quad (1)$$

If $m = n$, then by

$$A \begin{vmatrix} J \\ I \end{vmatrix} := \det A \begin{pmatrix} J \\ I \end{pmatrix} = A \begin{vmatrix} j_1, \dots, j_m \\ i_1, \dots, i_m \end{vmatrix},$$

we denote the determinant of $A \begin{pmatrix} J \\ I \end{pmatrix}$ which is called a *subdeterminant* of A . Throughout we set $A \begin{vmatrix} \emptyset \\ \emptyset \end{vmatrix} := 1$.

Let $N \in \mathbb{N}$, $I := (1, 2, \dots, N+1)$ and $I^\circ := (1, 2, \dots, N)$. By a prime we denote ordered complements with respect to I . Given elements f_1, \dots, f_N and $f := f_{N+1}$ of a linear space E over \mathbb{R} , elements L_1, \dots, L_N and $L := L_{N+1}$ of its dual E^* , consider the problem of finding

$$\langle L, p_1^N(f) \rangle, \quad (2)$$

where $p = p_1^N(f) = c_1 \cdot f_1 + \dots + c_N \cdot f_N$ satisfies the interpolation conditions

$$\langle L_i, p \rangle = \langle L_i, f \rangle \quad i \in I^\circ. \tag{3}$$

Here $\langle \cdot, \cdot \rangle$ means duality between E^* and E . If we write

$$A \begin{pmatrix} j \\ i \end{pmatrix} := \langle L_i, f_j \rangle \quad \text{for } i, j \in I, \quad (i, j) \neq (N + 1, N + 1),$$

and \mathbf{c} is the vector of components c_i , this problem is equivalent to solving the bordered system (cf. [16])

$$B \cdot \mathbf{x} = \mathbf{y} \quad \text{where } B = \begin{pmatrix} A \begin{pmatrix} I^\circ \\ I^\circ \end{pmatrix} & \mathbf{0} \\ A \begin{pmatrix} I^\circ \\ N + 1 \end{pmatrix} & 1 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} \mathbf{c} \\ \xi \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} A \begin{pmatrix} N + 1 \\ I^\circ \end{pmatrix} \\ A \begin{pmatrix} N + 1 \\ N + 1 \end{pmatrix} \end{pmatrix}. \tag{4}$$

Assuming $A \begin{pmatrix} I^\circ \\ I^\circ \end{pmatrix}$ nonsingular this can be solved by eliminating the components of \mathbf{c} in the last equation by adding a suitable linear combination of the first N equations of (4) to the last one, yielding one equation for one unknown, namely ξ :

$$\xi = A \begin{pmatrix} N + 1 \\ N + 1 \end{pmatrix} - A \begin{pmatrix} I^\circ \\ N + 1 \end{pmatrix} \cdot A \begin{pmatrix} I^\circ \\ I^\circ \end{pmatrix}^{-1} A \begin{pmatrix} N + 1 \\ I^\circ \end{pmatrix}. \tag{5}$$

Considering the effect of this block elimination step on the matrix

$$A = \begin{pmatrix} A \begin{pmatrix} I^\circ \\ I^\circ \end{pmatrix} & A \begin{pmatrix} N + 1 \\ I^\circ \end{pmatrix} \\ A \begin{pmatrix} I^\circ \\ N + 1 \end{pmatrix} & A \begin{pmatrix} N + 1 \\ N + 1 \end{pmatrix} \end{pmatrix}, \tag{6}$$

we find it transformed to

$$\tilde{A} = \begin{pmatrix} A \begin{pmatrix} I^\circ \\ I^\circ \end{pmatrix} & A \begin{pmatrix} N + 1 \\ I^\circ \end{pmatrix} \\ & \xi \end{pmatrix}.$$

If we take

$$A \begin{pmatrix} N + 1 \\ N + 1 \end{pmatrix} := 0, \tag{7}$$

then we have

$$\xi = -\langle L, p_1^N(f) \rangle. \tag{8}$$

On the other hand, if instead of (7) we take

$$A \begin{pmatrix} N + 1 \\ N + 1 \end{pmatrix} := \langle L_{N+1}, f_{N+1} \rangle, \tag{9}$$

then, in this frame, we get

$$\xi = \langle L, r_1^N(f) \rangle, \tag{10}$$

where

$$r_1^N(f) := f - p_1^N(f)$$

is the interpolation remainder.

If the systems (f_1, \dots, f_N) and (L_1, \dots, L_N) are independent of f and L then these problems are called *general linear extrapolation problems*, and if one or both do depend on $f = f_{N+1}$ or $L = L_{N+1}$ they are called problems of *quasilinear extrapolation*.

Observe, that with regard to determinants the block elimination step above is an elementary operation leaving the value of $\det A$ unchanged. Hence

$$\xi = \frac{\det A \begin{pmatrix} I \\ I \end{pmatrix}}{\det A \begin{pmatrix} I^\circ \\ I^\circ \end{pmatrix}},$$

which is known as the Schur complement of $A \begin{pmatrix} I \\ I^\circ \end{pmatrix}$ in $A \begin{pmatrix} I \\ I \end{pmatrix}$. This concept, introduced in [34,35] has found many applications in Linear Algebra and Statistics [13,53]. It may be generalized in different ways, see, for example, [21,22,44] where we used the concept of general elimination strategy which is explained in the next section.

3. Elimination strategies

In this section and the next two let $k, m, n \in \mathbb{N}$ such that $k + m = n$ and $I = (1, \dots, n)$. Given a square matrix $A = A \begin{pmatrix} I \\ I \end{pmatrix}$ over \mathbb{R} , how can we simplify $\det A$ by elementary operations, not altering the value of $\det A$, producing zeros in prescribed columns, e.g. in columns 1 to k ? Take a permutation of all rows, $M = (m_1, \dots, m_n)$ say, then look for a linear combination of k rows from (m_1, \dots, m_{n-1}) which, when added to row m_n , will produce zeros in columns 1 to k . Then add to row m_{n-1} a linear combination of k of its predecessors in M , to produce zeros in columns 1 to k , etc. Finally, add to row m_{k+1} a suitable linear combination of rows m_1, \dots, m_k to produce zeros in columns 1 to k . Necessarily,

$$A \left| \begin{array}{c} 1, \dots, k \\ j_1^r, \dots, j_k^r \end{array} \right| \neq 0$$

is assumed when a linear combination of rows j_1^r, \dots, j_k^r is added to row m_r ($r = n, n - 1, \dots, k + 1$) to generate zeros in columns 1 to k , and $j_q^r < m_r$ ($q = 1, \dots, k$; $r = n, n - 1, \dots, k + 1$) in order that in each step an elementary operation will be performed.

Let us give a formal description of this general procedure. Suppose that (I_s, I_s°) ($s = 1, \dots, m$) are pairs of ordered index lists of length $k + 1$ and k , respectively, over a basic index list M with $I_s^\circ \subset I_s$. Then the family

$$\Sigma := ((I_s, I_s^\circ))_{s=1, \dots, m}$$

will be called a (k, m) -elimination strategy over $I := I_1 \cup \dots \cup I_m$ provided that for $s = 2, \dots, m$

- (i) $\text{card}(I_1 \cup \dots \cup I_s) = k + s$,
- (ii) $I_s^\circ \subset I_s \cap (I_1 \cup \dots \cup I_{s-1})$.

By $E(k, m, I)$ we denote the set of all (k, m) -elimination strategies over I . $I^\circ := I_1^\circ$ is called the *basic index list* of the strategy Σ . For each s , the zeros in the row $\alpha_\Sigma(s) := I_s \setminus I_s^\circ$ are produced with the rows of I_s° . For shortness, we shall abbreviate the phrase “elimination strategy” by e.s. Notice that, when elimination is actually performed, it is done in the reverse ordering: first in row $\alpha_\Sigma(m)$, then in row $\alpha_\Sigma(m - 1)$, etc.

The simplest example of e.s. over $I = (1, \dots, m + k)$, is *Gauss elimination*:

$$\Gamma = ((G_s, G_s^\circ))_{s=1, \dots, m}, \quad G^\circ = G_s^\circ = \{1, \dots, k\}, \quad G_s = G^\circ \cup \{k + s\}. \tag{11}$$

For this strategy it is irrelevant in which order elimination is performed. This does not hold for another useful strategy over I :

$$\mathcal{N} = ((N_s, N_s^\circ))_{s=1, \dots, m} \tag{12}$$

with $N_s^\circ = (s, \dots, s + k - 1)$, $N_s = (s, \dots, s + k)$, $s = 1, \dots, m$, which we called [21,43,44] the *Neville* (k, m) -e.s. Using this strategy elimination must be performed from bottom to top. The reason for the name Neville is their relationship with Neville interpolation algorithm, based on consecutivity, see [43,23].

4. Generalized Schur complements

Suppose that $\Sigma = ((I_s, I_s^\circ))_{s=1, \dots, m} \in E(k, m, I)$ and that $\mathcal{K}^\circ \subset I$ is a fixed index list of length k . We assume that the submatrices $A \begin{pmatrix} \mathcal{K}^\circ \\ I_s^\circ \end{pmatrix}$ of a given matrix $A = A \begin{pmatrix} I \\ I \end{pmatrix} \in \mathbb{R}^{n \times n}$ are nonsingular for $s = 1, \dots, m$. Then the elimination strategy transforms A into the matrix \tilde{A} which, partitioned with respect to $I^\circ \cup I^{\circ'} = I$, $\mathcal{K}^\circ \cup \mathcal{K}^{\circ'} = I$, can be written as

$$\tilde{A} = \begin{pmatrix} \tilde{A} \begin{pmatrix} \mathcal{K}^\circ \\ I^\circ \end{pmatrix} & \tilde{A} \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^\circ \end{pmatrix} \\ 0 & \tilde{A} \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^{\circ'} \end{pmatrix} \end{pmatrix}$$

with

$$\tilde{A} \begin{pmatrix} \mathcal{K}^\circ \\ I^\circ \end{pmatrix} = A \begin{pmatrix} \mathcal{K}^\circ \\ I^\circ \end{pmatrix}, \quad \tilde{A} \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^\circ \end{pmatrix} = A \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^\circ \end{pmatrix}.$$

The submatrix $\tilde{S} := \tilde{A} \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^{\circ'} \end{pmatrix}$ of \tilde{A} is called the *Schur complement* of $A \begin{pmatrix} \mathcal{K}^\circ \\ I^\circ \end{pmatrix}$ in A with respect to the e.s. Σ and the column list \mathcal{K}° , and is also denoted by

$$\tilde{S} = \left[A \begin{pmatrix} I \\ I \end{pmatrix} / A \begin{pmatrix} \mathcal{K}^\circ \\ I^\circ \end{pmatrix} \right]_\Sigma.$$

When $\Sigma = \Gamma$ as in (11) and $\mathcal{K}^\circ = \{1, \dots, k\}$, then \tilde{S} is the classical Schur complement, which can also be written as

$$\tilde{A} \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^{\circ'} \end{pmatrix} = A \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^{\circ'} \end{pmatrix} - A \begin{pmatrix} \mathcal{K}^\circ \\ I^{\circ'} \end{pmatrix} A \begin{pmatrix} \mathcal{K}^\circ \\ I^\circ \end{pmatrix}^{-1} A \begin{pmatrix} \mathcal{K}^{\circ'} \\ I^\circ \end{pmatrix}.$$

When $\Sigma = \mathcal{N}$ is the Neville (k, m) -e.s. (12) and $\mathcal{K}^\circ = \{1, \dots, k\}$, then the rows of the Schur complement $\tilde{S} = \tilde{A}(\mathcal{K}^{\circ'})$ are

$$\tilde{A} \left(\begin{matrix} \mathcal{K}^{\circ'} \\ k+s \end{matrix} \right) = A \left(\begin{matrix} \mathcal{K}^{\circ'} \\ k+s \end{matrix} \right) - A \left(\begin{matrix} \mathcal{K}^\circ \\ k+s \end{matrix} \right) A \left(\begin{matrix} \mathcal{K}^\circ \\ s, \dots, s+k-1 \end{matrix} \right)^{-1} A \left(\begin{matrix} \mathcal{K}^{\circ'} \\ s, \dots, s+k-1 \end{matrix} \right) \quad s=1, \dots, m.$$

Whereas, the Schur complement of a submatrix depends essentially on the elimination strategies used, its determinant does not! There holds the following generalization of Schur’s classical determinantal identity [21,22,44]:

$$\det A \left(\begin{matrix} I \\ I \end{matrix} \right) = (-1)^\beta \det A \left(\begin{matrix} \mathcal{K}^\circ \\ I^\circ \end{matrix} \right) \det \left[A \left(\begin{matrix} I \\ I \end{matrix} \right) / A \left(\begin{matrix} \mathcal{K}^\circ \\ I^\circ \end{matrix} \right) \right]_\Sigma$$

for all e.s. $\Sigma \in E(k, m, I)$, where β is an integer depending only on Σ and \mathcal{K}° .

Also, Sylvester’s classical determinantal identity [55,56] has a corresponding generalization, see [18,21,22,43,44] for details. In the case of Gauss elimination we get Sylvester’s classical identity [9,10,55,56]

$$\det \left(A \left| \begin{matrix} 1, \dots, k, k+t \\ 1, \dots, k, k+s \end{matrix} \right. \right)_{s=1, \dots, m}^{t=1, \dots, m} = \det A \left(A \left| \begin{matrix} 1, \dots, k \\ 1, \dots, k \end{matrix} \right. \right)^{m-1}.$$

In the case of Neville elimination one has

$$\det \left(A \left| \begin{matrix} 1, \dots, k, k+t \\ s, \dots, s+k-1, s+k \end{matrix} \right. \right)_{s=1, \dots, m}^{t=1, \dots, m} = \det A \prod_{s=2}^m A \left| \begin{matrix} 1, \dots, k \\ s, \dots, s+k-1 \end{matrix} \right|.$$

Another identity of Sylvester’s type has been derived in [3]. Also some applications to the E -algorithm [5] are given there.

As we have seen, the technique of e.s. has led us in particular to general determinantal identities of Sylvester’s type. It can also be used to extend determinantal identities in the sense of Muir [51], see [47].

5. Application to quasilinear extrapolation problems

Suppose we are given elements f_1, \dots, f_N of a linear space E and elements L_1, \dots, L_N of its dual E^* . Consider furthermore elements $f =: f_{N+1}$ of E and $L =: L_{N+1}$ of E^* . Setting $I = (1, \dots, N+1)$, by A we denote the *generalized Vandermonde matrix*

$$A = A \left(\begin{matrix} I \\ I \end{matrix} \right) = V \left(\begin{matrix} f_1, \dots, f_N, f_{N+1} \\ L_1, \dots, L_N, L_{N+1} \end{matrix} \right) := (\langle L_i, f_j \rangle)_{i=1, \dots, N+1}^{j=1, \dots, N+1}. \tag{13}$$

Assume now that $k, m \in \mathbb{N}, m \leq N+1-k$ and that

$$\Sigma = ((I_s, I_s^\circ))_{s=1, \dots, m} \tag{14}$$

is a $(k-1, m)$ -e.s. over $\bigcup_{s=1}^m I_s \subset (1, \dots, N)$. Let $G := (1, \dots, k)$. If the submatrices

$$A \left(\begin{matrix} G \\ I_s \end{matrix} \right) \quad \text{are nonsingular for } s = 1, \dots, m, \tag{15}$$

then for $s = 1, \dots, m$ the interpolants

$$p_s^k(f) := \sum_{j=1}^k c_{s,j}^k(f) \cdot f_j, \tag{16}$$

satisfying the interpolation conditions

$$\langle L_i, p_s^k(f) \rangle = \langle L_i, f \rangle \quad \text{for } i \in I_s$$

are well defined as well as

$$\tau_s^k(f) := \langle L, p_s^k(f) \rangle.$$

Clearly, in case of general linear extrapolation the mapping

$$E \ni f \xrightarrow{p_s^k} p_s^k(f)$$

is a linear projection onto $\text{span}\{f_1, \dots, f_N\}$ and

$$E \ni f \xrightarrow{c_{s,j}^k} c_{s,j}^k(f)$$

is a linear functional. In case of quasilinear extrapolation we assume that, as a function of $f \in E$, p_s^k remains idempotent. Then, as a function of $f \in E$, in general the coefficients $c_{s,j}^k(f)$ are not linear. We assume that, as functions of $f \in \text{span}\{f_1, \dots, f_N\}$, $c_{s,j}^k(f)$ remain linear.

The task is

- (i) to find conditions, such that $p_1^N(f), \tau_1^N(f)$ are well defined, and
- (ii) to find methods to compute these quantities from $p_s^k(f), \tau_s^k(f) (s = 1, \dots, m)$, respectively.

When translated into pure terms of Linear Algebra these questions mean: Consider matrix (13) and assume (15),

- (i) under which conditions can we ensure that $A \begin{pmatrix} 1, \dots, N \\ 1, \dots, N \end{pmatrix}$ is nonsingular?

The coefficient problem reads:

- (ii') Suppose that we do know the solutions

$$\mathbf{c}_s^k(f) = (c_{s,j}^k(f))_{j=1, \dots, k}$$

of the linear systems

$$A \begin{pmatrix} G \\ I_s \end{pmatrix} \cdot \mathbf{c}_s^k(f) = A \begin{pmatrix} N+1 \\ I_s \end{pmatrix}, \quad s = 1, \dots, m.$$

How to get from these the solution $\mathbf{c}_1^N(f) = (c_{1,j}^N(f))_{j=1, \dots, N}$ of

$$A \begin{pmatrix} 1, \dots, N \\ 1, \dots, N \end{pmatrix} \cdot \mathbf{c}_1^N(f) = A \begin{pmatrix} N+1 \\ 1, \dots, N \end{pmatrix}?$$

The value problem reads:

- (iii) Suppose that we do know the values

$$\tau_s^k(f) = \langle L, p_s^k(f) \rangle, \quad s = 1, \dots, m.$$

How to get from these the value $\tau_1^N(f) = \langle L, p_1^N(f) \rangle$?

A dual coefficient problem can be also considered interchanging the roles of the spaces E and E^* . These problems were considered and solved in [20,7,19,31,40–42,45,48,50].

6. Applications to special classes of matrices

General elimination strategies, in particular the Neville e.s. and generalized Schur complements have found other applications in matrix theory and related problems.

In [21,22,44] we have considered some classes \mathcal{L}_n of real $n \times n$ -matrices A including the classes

- (i) \mathcal{C}_n of matrices satisfying $\det A \binom{J}{j} > 0$ for all $J \subset (1, \dots, n)$, $\det A \binom{K}{j} \cdot \det A \binom{J}{K} > 0$ for all $J, K \subset (1, \dots, n)$ of the same cardinality, which was considered in [36];
- (ii) of symmetric positive-definite matrices;
- (iii) of *strictly totally positive matrices* (STP), which are defined by the property that all square submatrices have positive determinants [36];
- (iv) of Minkowski matrices, defined by

$$A \binom{j}{i} < 0 \quad \text{for all } i \neq j, \quad \det A \binom{1, \dots, k}{1, \dots, k} > 0 \quad \text{for all } 1 \leq k \leq n.$$

In [21] we have proved that

$$A \in \mathcal{L}_n \Rightarrow \tilde{S} \in \mathcal{L}_m,$$

where $m = n - k$ and \tilde{S} denotes the classical Schur complement of $A \binom{1, \dots, k}{1, \dots, k}$ in A . For STP matrices also generalized Schur complements with respect to the Neville e.s. are STP. Using the Neville e.s. in [21,49] tests of algorithmic complexity $O(N^4)$ for matrices being STP were derived for the first time. Neville elimination, based on consecutivity, proved to be especially well suited for STP matrices, because these matrices were characterized in [36] by the property of having all subdeterminants with *consecutive* rows and columns positive.

Elimination by consecutive rows is not at all new in matrix theory. It has been used to prove some properties of special classes of matrices, for example, totally positive (TP) matrices, which, as it has already been said, are matrices with all subdeterminants nonnegative. However, motivated by the above mentioned algorithm for testing STP matrices, Gasca and Peña [24] initiated an exhaustive study of Neville elimination in an algorithmic way, of the pivots and multipliers used in the process to obtain new properties of totally positive matrices and to improve and simplify the known characterizations of these matrices.

Totally positive matrices have interesting applications in many fields, as, for example, vibrations of mechanical systems, combinatorics, probability, spline functions, computer-aided geometric design, etc., see [36,37]. For this reason, remarkable papers on total positivity due to specialists on these fields have appeared, see for example the ones collected in [29].

The important survey [2] presents a complete list of references on totally positive matrices before 1987. One of the main points in the recent study of this class of matrices has been that of characterizing them in practical terms, by factorizations or by the nonnegativity of some minors (instead of all of them, as claimed in the definition).

In [24] for example, it was proved that a matrix is STP if and only if all subdeterminants with lists of consecutive rows and consecutive columns, starting at least one of these lists by 1, are positive. Necessarily, one of the lists must start with 1. Observe, that the new characterization considerably decreases the number of subdeterminants to be checked, compared with the classical characterization, due to Fekete and Pólya [17], which used all subdeterminants with consecutive rows and columns.

This result means that the set of all subdeterminants of a matrix A with consecutive rows and columns, of the form

$$A \begin{vmatrix} 1, \dots, j \\ i, \dots, i+j-1 \end{vmatrix}, \quad A \begin{vmatrix} i, \dots, i+j-1 \\ 1, \dots, j \end{vmatrix},$$

called in [24] column- and row-initial minors, play in total positivity a similar role to that of the leading principal minors

$$A \begin{vmatrix} 1, \dots, j \\ 1, \dots, j \end{vmatrix}$$

in positive definiteness of symmetric real matrices. An algorithm based on Neville elimination was given in [24] with a complexity $O(N^3)$ for a matrix of order N , instead of the one with $O(N^4)$ previously obtained in [21,49]. Other similar simplifications were obtained in [24] for the characterization of totally positive matrices (not strictly).

Concerning factorizations, in [26] Neville elimination was described in terms of a product by bidiagonal unit-diagonal matrices. Some of the most well-known characterizations of TP and STP matrices are related to their LU factorization. Cryer [14,15], in the 1970s, extended to TP matrices what was previously known for STP matrices, thus obtaining the following result.

A square matrix A is TP (resp. STP) iff it has an LU factorization such that L and U are TP (Δ STP).

Here, as usual, L (resp. U) denotes a lower (upper) triangular matrix and Δ STP means triangular nonnegative matrices with all the nontrivial subdeterminants of any order strictly positive.

Also Cryer pointed out that the matrix A is STP iff it can be written in the form

$$A = \prod_{r=1}^N L_r \prod_{s=1}^M U_s$$

where each L_r (resp. U_s) is a lower (upper) Δ STP matrix. Observe that this result does not mention the relation of N or M with the order n of the matrix A .

The matricial description of Neville elimination obtained in [26] produced in the same paper the following result.

Let A be a nonsingular matrix of order n . Then A is STP iff it can be expressed in the form:

$$A = F_{n-1} \cdots F_1 D G_1 \cdots G_{n-1},$$

where, for each $i=1, 2, \dots, n-1$, F_i is a bidiagonal, lower triangular, unit diagonal matrix, with zeros in positions $(2, 1), \dots, (i, i-1)$ and positive entries in $(i+1, i), \dots, (n, n-1)$, G_i has the transposed form of F_i and D is a diagonal matrix with positive diagonal.

Similar results were obtained in [26] for TP matrices. In that paper all these new characterizations were collected in three classes: characterizations in terms of determinants, in terms of algorithms and in terms of factorizations.

7. Variation diminution and computer-aided geometric design

An $n \times n$ matrix A is said to be *sign-regular* (SR) if for each $1 \leq k \leq n$ all its minors of order k have the same (non strict) sign (in the sense that the product of any two of them is greater than or

equal to zero). The matrix is *strictly sign-regular* (SSR) if for each $1 \leq k \leq n$ all its minors of order k are different from zero and have the same sign. In [27] a test for strict sign regularity is given.

The importance of these types of matrices comes from their *variation diminishing properties*. By a *sign sequence* of a vector $x = (x_1, \dots, x_n)^T \in \mathbb{R}^n$ we understand any signature sequence ε for which $\varepsilon_i x_i = |x_i|$, $i = 1, 2, \dots, n$. The number of sign changes of x associated to ε , denoted by $\mathcal{C}(\varepsilon)$, is the number of indices i such that $\varepsilon_i \varepsilon_{i+1} < 0$, $1 \leq i \leq n-1$. The *maximum* (resp. *minimum*) *variation of signs*, $V_+(x)$ (resp. $V_-(x)$), is by definition the maximum (resp. minimum) of $\mathcal{C}(\varepsilon)$ when ε runs over all sign sequences of x . Let us observe that if $x_i \neq 0$ for all i , then $V_+(x) = V_-(x)$ and this value is usually called the exact variation of signs. The next result (see [2, Theorems 5.3 and 5.6]) characterizes sign-regular and strictly sign-regular matrices in terms of their variation diminishing properties.

Let A be an $n \times n$ nonsingular matrix. Then:

- (i) A is SR $\Leftrightarrow V_-(Ax) \leq V_-(x) \forall x \in \mathbb{R}^n$.
- (ii) A is SR $\Leftrightarrow V_+(Ax) \leq V_+(x) \forall x \in \mathbb{R}^n$.
- (iii) A is SSR $\Leftrightarrow V_+(Ax) \leq V_-(x) \forall x \in \mathbb{R}^n \setminus \{0\}$.

The above matricial definitions lead to the corresponding definitions for systems of functions. A system of functions (u_0, \dots, u_n) is *sign-regular* if all its collocation matrices are sign-regular of the same kind. The system is *strictly sign-regular* if all its collocation matrices are strictly sign-regular of the same kind. Here a *collocation matrix* is defined to be a matrix whose (i, j) -entry is of the form $u_i(x_j)$ with any system of strictly increasing points x_j .

Sign-regular systems have important applications in CAGD. Given u_0, \dots, u_n , functions defined on $[a, b]$, and $P_0, \dots, P_n \in \mathbb{R}^k$, we may define a curve $\gamma(t)$ by

$$\gamma(t) = \sum_{i=0}^n u_i(t) P_i.$$

The points P_0, \dots, P_n are called *control points*, because we expect to modify the shape of the curve by changing these points adequately. The polygon with vertices P_0, \dots, P_n is called *control polygon* of γ .

In CAGD the functions u_0, \dots, u_n are usually nonnegative and normalized ($\sum_{i=0}^n u_i(t) = 1 \forall t \in [a, b]$). In this case they are called *blending functions*. These requirements imply that the curve lies in the convex hull of the control polygon (*convex hull property*). Clearly, (u_0, \dots, u_n) is a system of blending functions if and only if all the collocation matrices are stochastic (that is, they are nonnegative matrices such that the elements of each row sum up to 1). For design purposes, it is desirable that the curve imitates the control polygon and that the control polygon even “exaggerates” the shape of the curve, and this holds when the system satisfies variation diminishing properties. If (u_0, \dots, u_n) is a sign-regular system of blending functions then the curve γ preserves many shape properties of the control polygon, due to the variation diminishing properties of (u_0, \dots, u_n) . For instance, any line intersects the curve no more often than it intersects the control polygon.

A characterization of SSR matrices A by the Neville elimination of A and of some submatrices of A is obtained in [26, Theorem 4.1].

A system of functions (u_0, \dots, u_n) is said to be *totally positive* if all its collocation matrices are totally positive. The system is *normalized totally positive* (NTP) if it is totally positive and $\sum_{i=0}^n u_i = 1$.

Normalized totally positive systems satisfy an interesting shape-preserving property, which is very convenient for design purposes and which we call *endpoint interpolation property*: the initial and final endpoints of the curve and the initial and final endpoints (respectively) of the control polygon coincide. In summary, these systems are characterized by the fact that they always generate curves γ satisfying simultaneously the convex hull, variation diminishing and endpoint interpolation properties.

Now the following question arises. Given a system of functions used in CAGD to generate curves, does there exist a basis of the space generated by that system with optimal shape preserving properties? Or equivalently, is there a basis such that the generated curves γ imitate better the form of the corresponding control polygon than the form of the corresponding control polygon for any other basis?

In the space of polynomials of degree less than or equal to n on a compact interval, the Bernstein basis is optimal. This was conjectured by Goodman and Said in [30], and it was proved in [11]. In [12], there is also an affirmative answer to the above questions for any space with TP basis. Moreover, Neville elimination provides a constructive way to obtain optimal bases. In the space of polynomial splines, B-splines form the optimal basis.

Since the product of TP matrices is a TP matrix, if (u_0, \dots, u_n) is a TP system of functions and A is a TP matrix of order $n+1$, then the new system $(u_0, \dots, u_n)A$ is again a TP system (which satisfies a “stronger” variation diminishing property than (u_0, \dots, u_n)). If we obtain from a basis (u_0, \dots, u_n) , in this way, all the totally positive bases of the space, then (u_0, \dots, u_n) will be the “least variation diminishing” basis of the space. In consequence, the control polygons with respect to (u_0, \dots, u_n) will imitate the form of the curve better than the control polygons with respect to other bases of the space. Therefore, we may reformulate the problem of finding an optimal basis (b_0, \dots, b_n) in the following way:

Given a vector space \mathcal{U} with a TP basis, is there a TP basis (b_0, \dots, b_n) of \mathcal{U} such that, for any TP basis (v_0, \dots, v_n) of \mathcal{U} there exists a TP matrix K satisfying $(v_0, \dots, v_n) = (b_0, \dots, b_n)K$?

The existence of such *optimal basis* (b_0, \dots, b_n) was proved in [12], where it was called *B-basis*. In the same paper, a method of construction, inspired by the Neville elimination process, was given. As mentioned above, Bernstein polynomials and B-splines are examples of B-bases.

Another point of view for B-bases is closely related to corner cutting algorithms, which play an important role in CAGD.

Given two NTP bases, (p_0, \dots, p_n) , (b_0, \dots, b_n) , let K be the nonsingular matrix such that

$$(p_0, \dots, p_n) = (b_0, \dots, b_n)K.$$

Since both bases are normalized, if K is a nonnegative matrix, it is clearly stochastic.

A curve γ can be expressed in terms of both bases

$$\gamma(t) = \sum_{i=0}^n B_i b_i(t) = \sum_{i=0}^n P_i p_i(t), \quad t \in [a, b],$$

and the matrix K gives the relationship between both control polygons

$$(B_0, \dots, B_n)^T = K(P_0, \dots, P_n)^T.$$

An *elementary corner cutting* is a transformation which maps any polygon $P_0 \cdots P_n$ into another polygon $B_0 \cdots B_n$ defined by:

$$\begin{aligned} B_j &= P_j, \quad j \neq i, \\ B_i &= (1 - \lambda)P_i + \lambda P_{i+1}, \quad \text{for one } i \in \{0, \dots, n-1\} \end{aligned} \quad (17)$$

or

$$\begin{aligned} B_j &= P_j, \quad j \neq i, \\ B_i &= (1 - \lambda)P_i + \lambda P_{i-1}, \quad \text{for one } i \in \{1, \dots, n\}. \end{aligned} \quad (18)$$

Here $\lambda \in (0, 1)$.

A *corner-cutting algorithm* is the algorithmic description of a corner cutting transformation, which is any composition of elementary corner cutting transformations.

Let us assume now that the matrix K above is TP. Since it is stochastic, nonsingular and TP, it can be factorized as a product of bidiagonal nonnegative matrices, (as we have mentioned in Section 6), which can be interpreted as a corner cutting transformation. Such factorizations are closely related to the Neville elimination of the matrix [28]. From the variation diminution produced by the totally positive matrices of the process, it can be deduced that the curve γ imitates better the form of the control polygon $B_0 \cdots B_n$ than that of the control polygon $P_0 \cdots P_n$. Therefore, we see again that an NTP basis (b_0, \dots, b_n) of a space \mathcal{U} has *optimal shape-preserving properties* if for any other NTP basis (p_0, \dots, p_n) of \mathcal{U} there exists a (stochastic) TP matrix K such that

$$(p_0, \dots, p_n) = (b_0, \dots, b_n)K. \quad (19)$$

Hence, a basis has optimal shape preserving properties if and only if it is a normalized B-basis. Neville elimination has also inspired the construction of B-bases in [11,12]. Many of these results and other important properties and applications of totally positive matrices have been collected, as we have already said in [28, Section 6].

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The epsilon algorithm and related topics

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Abstract

The epsilon algorithm is recommended as the best *all-purpose* acceleration method for slowly converging sequences. It exploits the numerical precision of the data to extrapolate the sequence to its limit. We explain its connections with Padé approximation and continued fractions which underpin its theoretical base. Then we review the most recent extensions of these principles to treat application of the epsilon algorithm to vector-valued sequences, and some related topics. In this paper, we consider the class of methods based on using generalised inverses of vectors, and the formulation specifically includes the complex case wherever possible. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Epsilon algorithm; qd algorithm; Padé; Vector-valued approximant; Wynn; Cross rule; Star identity; Compass identity; Designant

1. Introduction

A sequence with a limit is as basic a topic in mathematics as it is a useful concept in science and engineering. In the applications, it is usually the limit of a sequence, or a fixed point of its generator, that is required; the existence of the limit is rarely an issue, and rapidly convergent sequences are welcomed. However, if one has to work with a sequence that converges too slowly, the epsilon algorithm is arguably the best all-purpose method for accelerating its convergence. The algorithm was discovered by Wynn [54] and his review article [59] is highly recommended. The epsilon algorithm can also be used for weakly diverging sequences, and for these the desired limit is usually defined as being a fixed point of the operator that generates the sequence. There are interesting exceptional cases, such as quantum well oscillators [51], where the epsilon algorithm is not powerful enough and we refer to the companion paper by Homeier [33] in which the more

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powerful Levin-type algorithms, etc., are reviewed. The connections between the epsilon algorithm and similar algorithms are reviewed by Weniger [50,52].

This paper is basically a review of the application of the epsilon algorithm, with an emphasis on the case of complex-valued, vector-valued sequences. There are already many reviews and books which include sections on the scalar epsilon algorithm, for example [1,2,9,17,53]. In the recent past, there has been progress with the problem of numerical breakdown of the epsilon algorithm. Most notably, Cordellier's algorithm deals with both scalar and vector cases [13–16]. This work and its theoretical basis has been extensively reviewed [26,27]. In this paper, we focus attention on how the epsilon algorithm is used for sequences (s_i) in which $s_i \in \mathbb{C}^d$. The case $d = 1$ is the scalar case, and the formulation for $s_i \in \mathbb{C}$ is essentially the same as that for $s_i \in \mathbb{R}$. Not so for the vector case, and we give full details of how the vector epsilon and vector qd algorithms are implemented when $s_i \in \mathbb{C}^d$, and of the connections with vector Padé approximation. Understanding these connections is essential for specifying the range of validity of the methods. Frequently, the word “normally” appears in this paper to indicate that the results may not apply in degenerate cases. The adaptations for the treatment of degeneracy are almost the same for both real and complex cases, and so we refer to [25–27] for details.

In Section 2, we formulate the epsilon algorithm, and we explain its connection with Padé approximation and the continued fractions called C -fractions. We give an example of how the epsilon algorithm works in ideal circumstances, without any significant loss of numerical precision (which is an unusual outcome).

In Section 3, we formulate the vector epsilon algorithm, and we review its connection with vector-valued Padé approximants and with vector-valued C -fractions. There are two major generalisations of the scalar epsilon algorithm to the vector case. One of them is Brezinski's topological epsilon algorithm [5,6,35,48,49]. This algorithm has two principal forms, which might be called the forward and backward versions; and the backward version has the orthogonality properties associated with Lanczos methods [8]. The denominator polynomials associated with all forms of the topological epsilon algorithm have degrees which are the same as those for the scalar case [2,5,8]. By contrast, the other generalisation of the scalar epsilon algorithm to the vector case can be based on using generalised inverses of vectors, and it is this generalisation which is the main topic of this paper. We illustrate how the vector epsilon algorithm works in a two-dimensional real space, and we give a realistic example of how it works in a high-dimensional complex space. The denominator polynomials used in the scalar case are generalised both to operator polynomials of the same degree and to scalar polynomials of double the degree in the vector case, and we explain the connections between these twin generalisations. Most of the topics reviewed in Section 3 have a direct generalisation to the rational interpolation problem [25]. We also note that the method of GIPAs described in Section 3 generalises directly to deal with sequences of functions in $L_2(a, b)$ rather than vectors \mathbb{C}^d ; in this sense, the vectors are regarded as discretised functions [2].

In Section 4 we review the use of the vector qd algorithm for the construction of vector-valued C -fractions, and we note the connections between vector orthogonal polynomials and the vector epsilon algorithm. We prove the cross-rule (4.18), (4.22) using a Clifford algebra. For real-valued vectors, we observe that it is really an overlooked identity amongst Hankel designants. Here, the Cross Rule is proved as an identity amongst complex-valued vectors using Moore–Penrose inverses.

The importance of studying the vector epsilon algorithm lies partly in its potential [20] for application to the acceleration of convergence of iterative solution of discretised PDEs. For

example, Gauss–Seidel iteration generates sequences of vectors which often converge too slowly to be useful. *SOR*, multigrid and Lanczos methods are alternative approaches to the problem which are currently popular, but the success of the techniques like CGS and LTPMs (see [31] for an explanation of the techniques and the acronyms) indicates the need for continuing research into numerical methods for the acceleration of convergence of vector-valued sequences.

To conclude this introductory section, we recall that all algorithms have their domains of validity. The epsilon algorithm fails for logarithmically convergent sequences (which converge too slowly) and it fails to find the fixed point of the generator of sequences which diverge too fast. For example, if

$$s_n - s = \frac{C}{n} + O(n^{-2}), \quad C \neq 0,$$

the sequence (s_n) is logarithmically convergent to s . More precisely, a sequence is defined to converge logarithmically to s if it converges to s at a rate governed by

$$\lim_{n \rightarrow \infty} \frac{s_{n+1} - s}{s_n - s} = 1.$$

Not only does the epsilon algorithm usually fail for such sequences, but Delahaye and Germain-Bonne [18,19] have proved that there is no universal accelerator for logarithmically convergent sequences.

Reviews of series transformations, such as those of the energy levels of the quantum-mechanical harmonic oscillator [21,50,51], and of the Riemann zeta function [34], instructively show the inadequacy of the epsilon algorithm when the series coefficients diverge too fast. Information about the asymptotic form of the coefficients and scaling properties of the solution is exploited to create purpose-built acceleration methods. Exotic applications of the ε -algorithm appear in [55].

2. The epsilon algorithm

The epsilon algorithm was discovered by Wynn [54] as an efficient implementation of Shanks' method [47]. It is an algorithm for acceleration of convergence of a sequence

$$S = (s_0, s_1, s_2, \dots, s_i \in \mathbb{C}) \tag{2.1}$$

and it comprises the following initialisation and iterative phases:

Initialisation: For $j = 0, 1, 2, \dots$

$$\varepsilon_{-1}^{(j)} = 0 \quad (\text{artificially}), \tag{2.2}$$

$$\varepsilon_0^{(j)} = s_j. \tag{2.3}$$

Iteration: For $j, k = 0, 1, 2, \dots$

$$\varepsilon_{k+1}^{(j)} = \varepsilon_{k-1}^{(j+1)} + [\varepsilon_k^{(j+1)} - \varepsilon_k^{(j)}]^{-1}. \tag{2.4}$$

The entries $\varepsilon_k^{(j)}$ are displayed in the epsilon table on the left-hand side of Fig. 1, and the initialisation has been built in.

	s_0			4.000		
0	$\varepsilon_1^{(0)}$		0	-0.75		
	s_1	$\varepsilon_2^{(0)}$		2.667	3.167	
0	$\varepsilon_1^{(1)}$	\ddots	0	1.25	-28.75	
	s_2	$\varepsilon_2^{(1)}$		3.467	3.133	3.142
0	$\varepsilon_1^{(2)}$		0	-1.75	82.25	
	s_3	$\varepsilon_2^{(2)}$		2.895	3.145	
0	\vdots	\ddots	0	2.25		
	\vdots					

Fig. 1. The epsilon table, and a numerical example of it.

Example 2.1. Gregory’s series for $\tan^{-1} z$ is

$$\tan^{-1} z = z - \frac{z^3}{3} + \frac{z^5}{5} - \frac{z^7}{7} + \dots \tag{2.5}$$

This series can be used to determine the value of π by evaluating its MacLaurin sections at $z = 1$:

$$s_j := [4 \tan^{-1}(z)]_0^{2j+1} \Big|_{z=1}, \quad j = 0, 1, 2, \dots \tag{2.6}$$

Nuttall’s notation is used here and later on. For a function whose MacLaurin series is

$$\phi(z) = \phi_0 + \phi_1 z + \phi_2 z^2 + \dots,$$

its sections are defined by

$$[\phi(z)]_j^k = \sum_{i=j}^k \phi_i z^i \quad \text{for } 0 \leq j \leq k. \tag{2.7}$$

In fact, $s_j \rightarrow \pi$ as $j \rightarrow \infty$ [2] but sequence (2.6) converges slowly, as is evidenced in the column $k = 0$ of entries $s_j = \varepsilon_0^{(j)}$ in Fig. 1. The columns of odd index have little significance, whereas the columns of even index can be seen to converge to π , which is the correct limit [2], increasingly fast, as far as the table goes. Some values of $\varepsilon_{2k}^{(j)}$ are also shown on the bar chart (Fig. 2). Notice that $\varepsilon_2^{(2)} = 3.145$ and $\varepsilon_4^{(0)} = 3.142$ cannot be distinguished visually on this scale.

In Example 2.1, convergence can be proved and the rate of convergence is also known [2]. From the theoretical viewpoint, Example 2.1 is ideal for showing the epsilon algorithm at its best. It is noticeable that the entries in the columns of odd index are large, and this effect warns us to beware of possible loss of numerical accuracy. Like all algorithms of its kind (which use reciprocal differences of convergent sequences) the epsilon algorithm uses (and usually uses up) numerical precision of the data to do its extrapolation. In this case, there is little loss of numerical precision using 16 decimal place (MATLAB) arithmetic, and $\varepsilon_{22}^{(0)} = \pi$ almost to machine precision. In this case, the epsilon algorithm converges with great numerical accuracy because series (2.5) is a totally oscillating series [4,7,17,59].

To understand in general how and why the epsilon algorithm converges, whether we are referring to its even columns ($\varepsilon_{2k}^{(j)}$, $j = 0, 1, 2, \dots, k$ fixed) or its diagonals ($\varepsilon_{2k}^{(j)}$, $k = 0, 1, 2, \dots, j$ fixed) or any

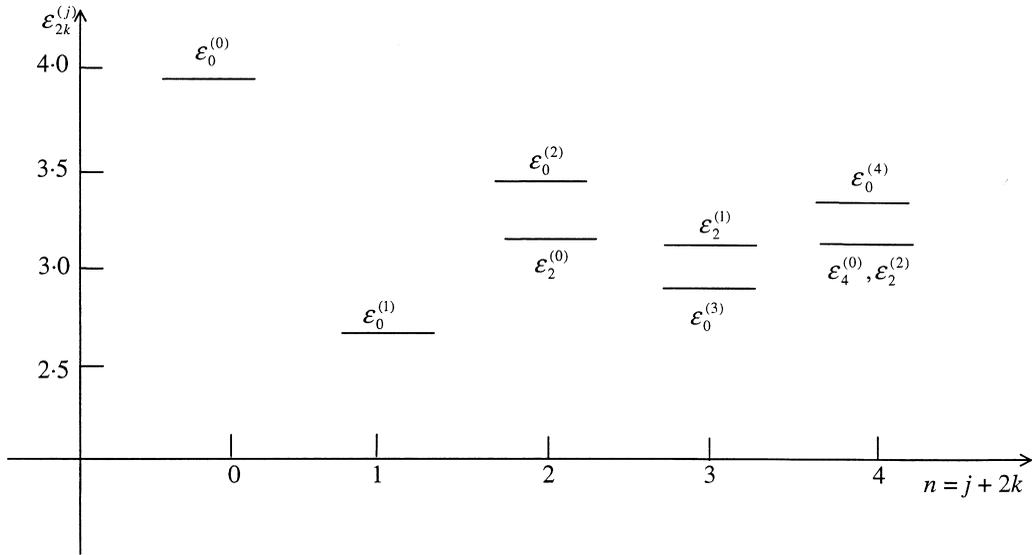


Fig. 2. Values of $\varepsilon_{2k}^{(j)}$ for Example 2.1, showing the convergence rate of the epsilon algorithm using $n + 1 = 1, 2, 3, 4, 5$ terms of the given sequence.

other sequence, the connection with Padé approximation is essential [1,2,56]. Given a (possibly formal) power series

$$f(z) = c_0 + c_1z + c_2z^2 + \dots, \tag{2.8}$$

the rational function

$$A(z)B(z)^{-1} \equiv [\ell/m](z) \tag{2.9}$$

is defined as a Padé approximant for $f(z)$ of type $[\ell/m]$ if

$$(i) \text{deg}\{A(z)\} \leq \ell, \quad \text{deg}\{B(z)\} \leq m, \tag{2.10}$$

$$(ii) f(z)B(z) - A(z) = O(z^{\ell+m+1}), \tag{2.11}$$

$$(iii) B(0) \neq 0. \tag{2.12}$$

The Baker condition

$$B(0) = 1 \tag{2.13}$$

is often imposed for reliability in the sense of (2.14) below and for a definite specification of $A(z)$ and $B(z)$. The definition above contrasts with the classical (Frobenius) definition in which axiom (iii) is waived, and in this case the existence of $A(z)$ and $B(z)$ is guaranteed, even though (2.14) below is not. Using specification (2.10)–(2.13), we find that

$$f(z) - A(z)B(z)^{-1} = O(z^{\ell+m+1}), \tag{2.14}$$

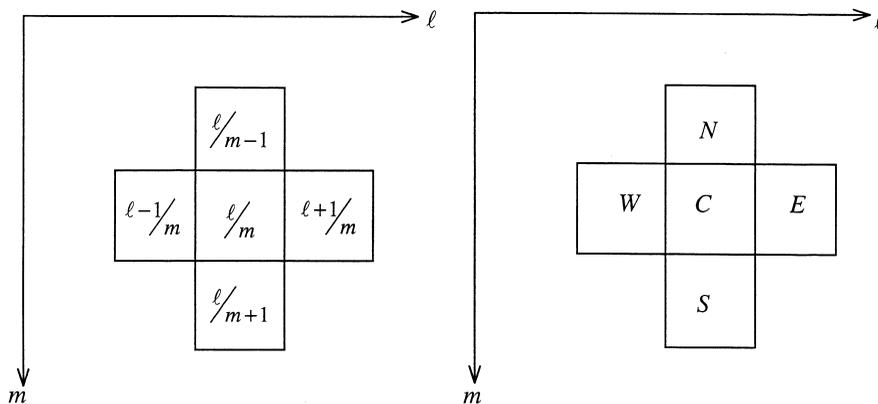


Fig. 3. Relative location of Padé approximants.

provided that a solution of (2.15) below can be found. To find $B(z)$, the linear equations corresponding to accuracy-through-orders $z^{\ell+1}, z^{\ell+2}, \dots, z^{\ell+m}$ in (2.11) must be solved. They are

$$\begin{bmatrix} c_{\ell-m+1} & \dots & c_{\ell} \\ \vdots & & \vdots \\ c_{\ell} & \dots & c_{\ell+m-1} \end{bmatrix} \begin{bmatrix} b_m \\ \vdots \\ b_1 \end{bmatrix} = - \begin{bmatrix} c_{\ell+1} \\ \vdots \\ c_{\ell+m} \end{bmatrix}. \tag{2.15}$$

The coefficients of $B(z) = \sum_{i=0}^m b_i z^i$ are found using an accurate numerical solver of (2.15). By contrast, for purely theoretical purposes, Cramer’s rule is applied to (2.15). We are led to define

$$q^{[\ell/m]}(z) = \begin{vmatrix} c_{\ell-m+1} & c_{\ell-m+2} & \dots & c_{\ell+1} \\ c_{\ell-m+2} & c_{\ell-m+3} & \dots & c_{\ell+2} \\ \vdots & \vdots & & \vdots \\ c_{\ell} & c_{\ell+1} & \dots & c_{\ell+m} \\ z^m & z^{m-1} & \dots & 1 \end{vmatrix} \tag{2.16}$$

and then we find that

$$B^{[\ell/m]}(z) = q^{[\ell/m]}(z)/q^{[\ell/m]}(0) \tag{2.17}$$

is the denominator polynomial for the Padé approximation problem (2.9)–(2.15) provided that $q^{[\ell/m]}(0) \neq 0$.

The collection of Padé approximants is called the Padé table, and in Fig. 3 we show five neighbouring approximants in the table.

These approximants satisfy a five-point star identity,

$$[N(z) - C(z)]^{-1} + [S(z) - C(z)]^{-1} = [E(z) - C(z)]^{-1} + [W(z) - C(z)]^{-1}, \tag{2.18}$$

called Wynn’s identity or the compass identity. The proof of (2.18) is given in [1,2], and it is also a corollary (in the case $d = 1$) of the more general result (3.59) that we prove in the next section. Assuming (2.18) for the moment, the connection between Padé approximation and the epsilon

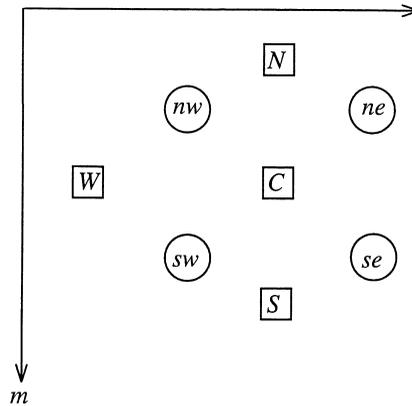


Fig. 4. Some artificial entries in the Padé table are shown circled.

algorithm is given by connecting the coefficients of $f(z)$ with those of S with

$$c_0 = s_0, \quad c_i = s_i - s_{i-1}, \quad i = 1, 2, 3, \dots,$$

and by

Theorem 2.1. *The entries in columns of even index in the epsilon table are values of Padé approximants given by*

$$\varepsilon_{2k}^{(j)} = [j + k/k](1) \tag{2.19}$$

provided (i) zero divisors do not occur in the construction of the epsilon table, and (ii) the corresponding Padé approximants identified by (2.19) exist.

Proof. The entries W, C, E in the Padé table of Figs. 3 and 4 may be taken to correspond to entries $\varepsilon_{2k}^{(j-1)}, \varepsilon_{2k}^{(j)}, \varepsilon_{2k}^{(j+1)}$, respectively, in the epsilon table. They neighbour other elements in columns of odd index in the epsilon table, $nw := \varepsilon_{2k-1}^{(j)}$, $ne := \varepsilon_{2k-1}^{(j+1)}$, $se := \varepsilon_{2k+1}^{(j)}$ and $sw := \varepsilon_{2k+1}^{(j-1)}$. By re-pairing, we have

$$(nw - sw) - (ne - se) = (nw - ne) - (sw - se). \tag{2.20}$$

By applying the epsilon algorithm to each term in (2.20), we obtain the compass identity (2.18). □

With our conventions, the approximants of type $[\ell/0]$ lie in the first row ($m = 0$) of the Padé table. This is quite natural when we regard these approximants as MacLaurin sections of $f(z)$. However, it must be noted that the row sequence ($[\ell/m](1), \ell = m + j, m + j + 1, \dots, m$ fixed) corresponds to the column sequence of entries ($\varepsilon_{2m}^{(j)}, j = 0, 1, 2, \dots, m$ fixed); this identification follows from (2.19).

A key property of Padé approximants that is an axiom of their definition is that of accuracy-through-order, also called correspondence. Before Padé approximants were known as such, attention had rightly been focused on the particular sequence of rational fractions which are truncations of the

continued fraction

$$f(z) = \frac{c_0}{1} - \frac{za_1}{1} - \frac{za_2}{1} - \frac{za_3}{1} - \dots \tag{2.21}$$

The right-hand side of (2.21) is called a *C*-fraction (for instance, see [36]), which is short for corresponding fraction, and its truncations are called its convergents. Normally, it can be constructed by successive reciprocation and re-expansion. The first stage of this process is

$$\frac{1 - c_0/f(z)}{z} = \frac{a_1}{1} - \frac{za_2}{1} - \frac{za_3}{1} - \dots \tag{2.22}$$

By undoing this process, we see that the convergents of the *C*-fraction are rational fractions in the variable *z*.

By construction, we see that these convergents agree order by order with *f*(*z*), provided all *a_i* ≠ 0, and this property is called correspondence.

Example 2.2. We truncate (2.21) after *a₂* and obtain

$$\frac{A_2(z)}{B_2(z)} = \frac{c_0}{1} - \frac{za_1}{1 - za_2} \tag{2.23}$$

This is a rational fraction of type [1/1], and we take

$$A_2(z) = c_0(1 - za_2), \quad B_2(z) = 1 - z(a_1 + a_2).$$

Provided all the *a_i* ≠ 0, the convergents of (2.21) are well defined. The equality in (2.21) is not to be understood in the sense of pointwise convergence for each value of *z*, but in the sense of correspondence order by order in powers of *z*.

The numerators and denominators of the convergents of (2.21) are usually constructed using Euler’s recursion. It is initialised, partly artificially, by

$$A_{-1}(z) = 0, \quad A_0(z) = c_0, \quad B_{-1}(z) = 1, \quad B_0(z) = 1 \tag{2.24}$$

and the recursion is

$$A_{i+1}(z) = A_i(z) - a_{i+1}zA_{i-1}(z), \quad i = 0, 1, 2, \dots, \tag{2.25}$$

$$B_{i+1}(z) = B_i(z) - a_{i+1}zB_{i-1}(z), \quad i = 0, 1, 2, \dots \tag{2.26}$$

Euler’s formula is proved in many texts, for example, [1,2,36]. From (2.24) to (2.26), it follows by induction that

$$\ell = \deg\{A_i(z)\} \leq \left\lfloor \frac{i}{2} \right\rfloor, \quad m = \deg\{B_i(z)\} \leq \left\lfloor \frac{i+1}{2} \right\rfloor, \tag{2.27}$$

where [·] represents the integer part function and the Baker normalisation is built in:

$$B_i(0) = 1, \quad i = 0, 1, 2, \dots \tag{2.28}$$

The sequence of approximants generated by (2.24)–(2.26) is shown in Fig. 5.

From (2.19) and (2.27), we see that the convergents of even index *i* = 2*k* correspond to Padé approximants of type [k/k]; when they are evaluated at *z* = 1, they are values of ε_{2k}⁽⁰⁾ on the leading diagonal of the epsilon table.

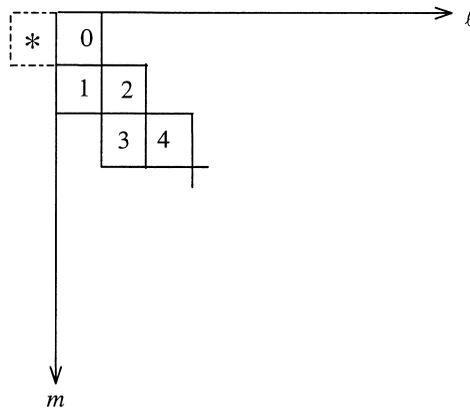


Fig. 5. A staircase sequence of approximants indexed by i , as in (2.27).

The epsilon algorithm was introduced in (2.1)–(2.4) as a numerical algorithm. Eq. (2.19) states its connection with values of certain Padé approximants. However, the epsilon algorithm can be given a symbolic interpretation if it is initialised with

$$\varepsilon_{-1}^{(j)} = 0, \quad \varepsilon_0^{(j)} = \sum_{i=0}^j c_i z^i \tag{2.29}$$

instead of (2.2) and (2.3). In this case, (2.19) would become

$$\varepsilon_{2k}^{(j)}(z) = [j + k/k](z). \tag{2.30}$$

The symbolic implementation of the iterative process (2.4) involves considerable cancellation of polynomial factors, and so we regard this procedure as being primarily of conceptual value.

We have avoided detailed discussions of normality and degeneracy [1,2,25] in this paper so as to focus on the algorithmic aspects. The case of numerical breakdown associated with zero divisors is treated by Cordellier [14,15] for example. Refs. [1,2] contain formulae for the difference between Padé approximants occupying neighbouring positions in the Padé table. Using these formulae, one can show that condition (i) of Theorem 2.1 implies that condition (ii) holds, and so conditions (ii) can be omitted.

It is always worthwhile to consider the case in which an approximation method gives exact results at an intermediate stage so that the algorithm is terminated at that stage. For example, let

$$f(z) = v_0 + \sum_{\kappa=1}^k \frac{v_\kappa}{1 - z\theta_\kappa} \tag{2.31}$$

with $v_\kappa, \theta_\kappa \in \mathbb{C}$, each $|\theta_\kappa| < 1$, each $v_\kappa \neq 0$ and all θ_κ distinct. Then $f(z)$ is a rational function of precise type $[k/k]$. It is the generating function of the generalised geometric sequence S with elements

$$s_j = v_0 + \sum_{\kappa=1}^k v_\kappa \frac{1 - \theta_\kappa^{j+1}}{1 - \theta_\kappa}, \quad j = 0, 1, 2, \dots \tag{2.32}$$

This sequence is sometimes called a Dirichlet series and it converges to $s_\infty = f(1)$ as $j \rightarrow \infty$. Its elements can also be expressed as

$$s_j = s_\infty - \sum_{\kappa=1}^k w_\kappa \theta_\kappa^j \tag{2.33}$$

if

$$s_\infty = \sum_{\kappa=0}^k v_\kappa + \sum_{\kappa=1}^k w_\kappa \quad \text{and} \quad w_\kappa = \theta_\kappa v_\kappa (1 - \theta_\kappa)^{-1}.$$

Then (2.33) expresses the fact that S is composed of exactly k non-trivial, distinct geometric components. Theorem 2.1 shows that the epsilon algorithm yields

$$\varepsilon_{2k}^{(j)} = s_\infty, \quad j = 0, 1, 2, \dots$$

which is the ‘exact result’ in each row of the column of index $2k$, provided that zero divisors have not occurred before this column is constructed. The algorithm should be terminated at this stage via a consistency test, because zero divisors necessarily occur at the next step. Remarkably, the epsilon algorithm has some smoothing properties [59], which may (or may not) disguise this problem when rounding errors occur.

In the next sections, these results will be generalised to the vector case. To do that, we will also need to consider the paradiagonal sequences of Padé approximants given by $([m + J/m](z), m = 0, 1, 2, \dots, J \geq 0, J \text{ fixed})$. After evaluation at $z = 1$, we find that this is a diagonal sequence $(\varepsilon_{2m}^{(J)}, m = 0, 1, 2, \dots, J \geq 0, J \text{ fixed})$ in the epsilon table.

3. The vector epsilon algorithm

The epsilon algorithm acquired greater interest when Wynn [57,58] showed that it has a useful and immediate generalisation to the vector case. Given a sequence

$$\mathbf{S} = (s_0, s_1, s_2, \dots : s_i \in \mathbb{C}^d), \tag{3.1}$$

the standard implementation of the vector epsilon algorithm (VEA) consists of the following initialisation from \mathbf{S} followed by its iteration phase:

Initialisation: For $j = 0, 1, 2, \dots$,

$$\varepsilon_{-1}^{(j)} = \mathbf{0} \quad (\text{artificially}), \tag{3.2}$$

$$\varepsilon_0^{(j)} = \mathbf{s}_j. \tag{3.3}$$

Iteration: For $j, k = 0, 1, 2, \dots$,

$$\varepsilon_{k+1}^{(j)} = \varepsilon_{k-1}^{(j+1)} + [\varepsilon_k^{(j+1)} - \varepsilon_k^{(j)}]^{-1}. \tag{3.4}$$

The iteration formula (3.4) is identical to (2.4) for the scalar case, except that it requires the specification of an inverse (reciprocal) of a vector. Usually, the Moore–Penrose (or Samelson) inverse

$$\mathbf{v}^{-1} = \mathbf{v}^* / (\mathbf{v}^H \mathbf{v}) = \mathbf{v}^* / \sum_{i=1}^d |v_i|^2 \tag{3.5}$$

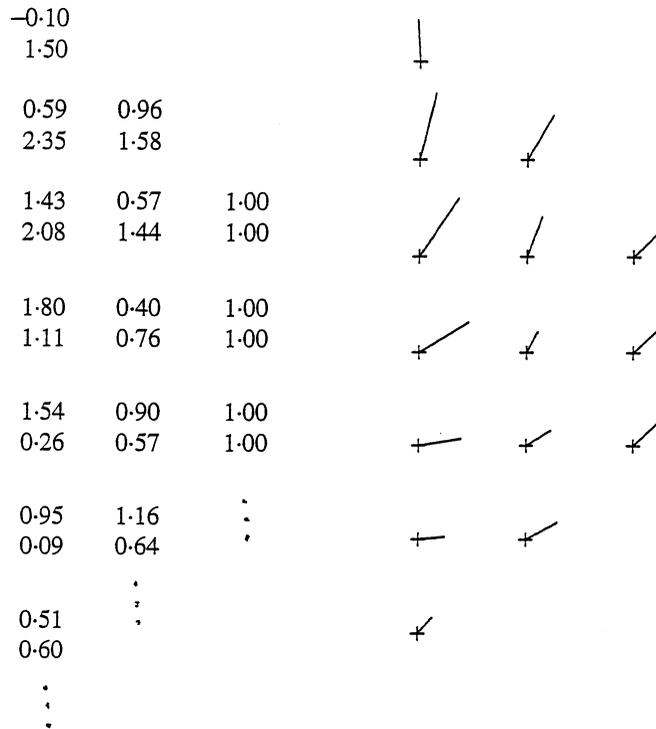


Fig. 6. Columns $k = 0, 2$ and 4 of the vector epsilon table for Example 3.1 are shown numerically and graphically.

(where the asterisk denotes the complex conjugate and H the Hermitian conjugate) is the most useful, but there are exceptions [39]. In this paper, the vector inverse is defined by (3.5). The vector epsilon table can then be constructed column by column from (3.2) to (3.4), as in the scalar case, and as shown in Fig. 6.

Example 3.1. The sequence S is initialised by

$$s_0 := \mathbf{b} := (-0.1, 1.5)^T \tag{3.6}$$

(where T denotes the transpose) and it is generated recursively by

$$s_{j+1} := \mathbf{b} + Gs_j, \quad j = 0, 1, 2, \dots \tag{3.7}$$

with

$$G = \begin{bmatrix} 0.6 & 0.5 \\ -1 & 0.5 \end{bmatrix}. \tag{3.8}$$

The fixed point of (3.7) is $\mathbf{x} = [1, 1]$, which is the solution of $A\mathbf{x} = \mathbf{b}$ with $A = I - G$.

Notice that

$$\varepsilon_4^{(j)} = \mathbf{x} \quad \text{for } j = 0, 1, 2$$

and this ‘exact’ result is clearly demonstrated in the right-hand columns of Fig. 6.

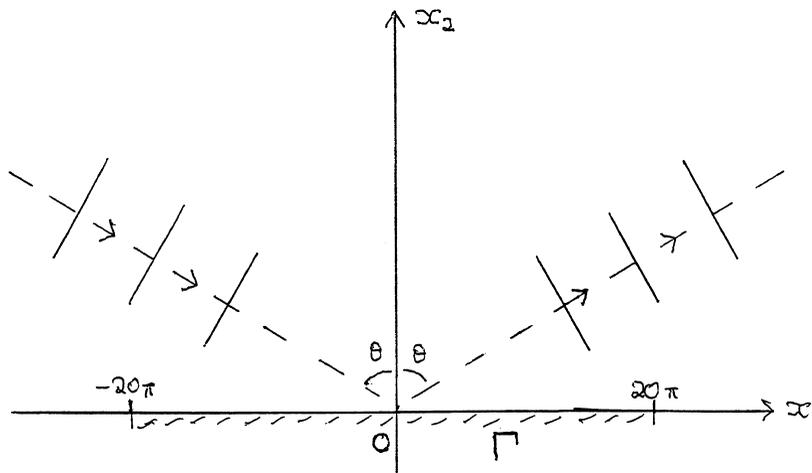


Fig. 7. Schematic view of the two components of $u_1(\mathbf{x})$ and the boundary Γ on the x_1 -axis.

This elementary example demonstrates how the VEA can be a powerful convergence accelerator in an ideal situation. With the same rationale as was explained in the scalar case, the vector epsilon algorithm is used for sequences of vectors when their convergence is too slow. Likewise, the VEA can find an accurate solution (as a fixed point of an associated matrix operator) even when the sequence of vectors is weakly divergent. In applications, these vector sequences usually arise as sequences of discretised functions, and the operator is a (possibly nonlinear) integral operator. An example of this kind of vector sequence is one that arises in a problem of current interest. We consider a problem in acoustics, which is based on a boundary integral equation derived from the Helmholtz equation [12]. Our particular example includes impedance boundary conditions (3.12) relevant to the design of noise barriers.

Example 3.2. This is an application of the VEA for the solution of

$$u(\mathbf{x}) = u_1(\mathbf{x}) + ik \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) [\beta(\mathbf{y}) - 1] u(\mathbf{y}) d\mathbf{y} \quad (3.9)$$

for the acoustic field $u(\mathbf{x})$ at the space point $\mathbf{x} = (x_1, x_2)$. This field is confined to the half-space $x_2 \geq 0$ by a barrier shown in Fig. 7. The inhomogeneous term in (3.9) is

$$u_1(\mathbf{x}) = e^{ik(x_1 \sin \theta - x_2 \cos \theta)} + R e^{ik(x_1 \sin \theta + x_2 \cos \theta)} \quad (3.10)$$

which represents an incoming plane wave and a “partially reflected” outgoing plane wave with wave number k . The reflection coefficient in (3.10) is given by

$$R = -\tan^2 \left(\frac{\theta}{2} \right), \quad (3.11)$$

so that $u_1(\mathbf{x})$ and $u(\mathbf{x})$ satisfy the impedance boundary conditions

$$\frac{\partial u_1}{\partial x_2} = -iku_1 \quad \text{and} \quad \frac{\partial u}{\partial x_2} = -ik\beta u \quad \text{on } \Gamma. \quad (3.12)$$

Notice that $u(x_1, 0) = u_1(x_1, 0)$ if $\beta(x_1, 0) \equiv 1$. Then a numerically useful form of the Green’s function in (3.9) is [10]

$$G(\mathbf{x}, \mathbf{y}) = \frac{i}{2} H_0^{(1)}(kr) + \frac{e^{ikr}}{\pi} \int_0^\infty \frac{t^{-1/2} e^{-krt} (1 + \gamma + \gamma it)}{\sqrt{t - 2i(t - i - i\gamma)^2}} dt, \tag{3.13}$$

where $\mathbf{w} = \mathbf{x} - \mathbf{y}$, $r = |\mathbf{w}|$, $\gamma = w_2/r$ and $H_0^{(1)}(z)$ is a Hankel function of the first kind, as specified more fully in [10,11]. By taking $x_2 = 0$ in (3.9), we see from (3.13) that $u(x_1, 0)$ satisfies an integral equation with Toeplitz structure, and the fast Fourier transform yields its iterative solution efficiently.

Without loss of generality, we use the scale determined by $k=1$ in (3.9)–(3.13). For this example, the impedance is taken to be $\beta = 1.4e^{i\pi/4}$ on the interval $\Gamma = \{\mathbf{x}: -40\pi < x_1 < 40\pi, x_2 = 0\}$. At two sample points ($x_1 \approx -20\pi$ and 20π) taken from a 400-point discretisation of Γ , we found the following results with the VEA using 16 decimal place (MATLAB) arithmetic

$$\begin{aligned} \varepsilon_0^{(12)} &= [\dots, -\mathbf{0.36843} + \mathbf{0.44072i}, \dots, -\mathbf{0.14507} + \mathbf{0.55796i}, \dots], \\ \varepsilon_2^{(10)} &= [\dots, -\mathbf{0.36333} + \mathbf{0.45614i}, \dots, -\mathbf{0.14565} + \mathbf{0.56342i}, \dots], \\ \varepsilon_4^{(8)} &= [\dots, -\mathbf{0.36341} + \mathbf{0.45582i}, \dots, -\mathbf{0.14568} + \mathbf{0.56312i}, \dots], \\ \varepsilon_6^{(6)} &= [\dots, -\mathbf{0.36341} + \mathbf{0.45583i}, \dots, -\mathbf{0.14569} + \mathbf{0.56311i}, \dots], \\ \varepsilon_8^{(4)} &= [\dots, -\mathbf{0.36341} + \mathbf{0.45583i}, \dots, -\mathbf{0.14569} + \mathbf{0.56311i}, \dots], \end{aligned}$$

where the converged figures are shown in bold face.

Each of these results, showing just two of the components of a particular $\varepsilon_\kappa^{(j)}$ in columns $\kappa = 0, 2, \dots, 8$ of the vector-epsilon table, needs 12 iterations of (3.9) for its construction. In this application, these results show that the VEA converges reasonably steadily, in contrast to Lanczos type methods, eventually yielding five decimal places of precision.

Example 3.2 was chosen partly to demonstrate the use of the vector epsilon algorithm for a weakly convergent sequence of complex-valued data, and partly because the problem is one which lends itself to iterative methods. In fact, the example also shows that the VEA has used up 11 of the 15 decimal places of accuracy of the data to extrapolate the sequence to its limit. If greater precision is required, other methods such as stabilised Lanczos or multigrid methods should be considered.

The success of the VEA in examples such as those given above is usually attributed to the fact that the entries $\{\varepsilon_{2k}^{(j)}, j = 0, 1, 2, \dots\}$ are the exact limit of a convergent sequence S if S is generated by precisely k nontrivial geometric components. This result is an immediate and direct generalisation of that for the scalar case given in Section 2. The given vector sequence is represented by

$$s_j = \mathbf{v}_0 + \sum_{\kappa=1}^k \mathbf{v}_\kappa \sum_{i=0}^j (\theta_\kappa)^i = \mathbf{s}_\infty - \sum_{\kappa=1}^k \mathbf{w}_\kappa (\theta_\kappa)^j, \quad j = 0, 1, 2, \dots, \tag{3.14}$$

where each $\mathbf{v}_\kappa, \mathbf{w}_\kappa \in \mathbb{C}^d$, $\theta_\kappa \in \mathbb{C}$, $|\theta_\kappa| < 1$, and all the θ_κ are distinct. The two representations used in (3.14) are consistent if

$$\sum_{\kappa=0}^k \mathbf{v}_\kappa = \mathbf{s}_\infty - \sum_{\kappa=1}^k \mathbf{w}_\kappa \quad \text{and} \quad \mathbf{v}_\kappa = \mathbf{w}_\kappa (\theta_\kappa^{-1} - 1).$$

To establish this convergence result, and its generalisations, we must set up a formalism which allows vectors to be treated algebraically.

From the given sequence $\mathbf{S} = (s_i, i = 0, 1, 2, \dots, : s_i \in \mathbb{C}^d)$, we form the series coefficients

$$\mathbf{c}_0 := s_0, \quad \mathbf{c}_i := s_i - s_{i-1}, \quad i = 1, 2, 3, \dots \tag{3.15}$$

and the associated generating function

$$\mathbf{f}(z) = \mathbf{c}_0 + \mathbf{c}_1 z + \mathbf{c}_2 z^2 + \dots \in \mathbb{C}^d[[z]]. \tag{3.16}$$

Our first aim is to find an analogue of (2.15) which allows construction, at least in principle, of the denominator polynomials of a vector-valued Padé approximant for $\mathbf{f}(z)$. This generalisation is possible if the vectors \mathbf{c}_j in (3.16) are put in one–one correspondence with operators c_j in a Clifford algebra \mathcal{A} . The details of how this is done using an explicit matrix representation were basically set out by McLeod [37]. We use his approach [26,27,38] and square matrices $E_i, i = 1, 2, \dots, 2d + 1$ of dimension 2^{2d+1} which obey the anticommutation relations

$$E_i E_j + E_j E_i = 2\delta_{ij} I, \tag{3.17}$$

where I is an identity matrix. The special matrix $J = E_{2d+1}$ is used to form the operator products

$$F_i = J E_{d+i}, \quad i = 1, 2, \dots, d. \tag{3.18}$$

Then, to each vector $\mathbf{w} = \mathbf{x} + i\mathbf{y} \in \mathbb{C}^d$ whose real and imaginary parts $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, we associate the operator

$$w = \sum_{i=1}^d x_i E_i + \sum_{i=1}^d y_i F_i. \tag{3.19}$$

The real linear space \mathcal{V} is defined as the set of all elements of the form (3.19). If $w_1, w_2 \in \mathcal{V}$ correspond to $\mathbf{w}_1, \mathbf{w}_2 \in \mathbb{C}^d$ and α, β are real, then

$$w_3 = \alpha w_1 + \beta w_2 \in \mathcal{V} \tag{3.20}$$

corresponds uniquely to $\mathbf{w}_3 = \alpha \mathbf{w}_1 + \beta \mathbf{w}_2 \in \mathbb{C}^d$. Were α, β complex, the correspondence would not be one–one. We refer to the space \mathcal{V} as the isomorphic image of \mathbb{C}^d , where the isomorphism preserves linearity only in respect of real multipliers as shown in (3.20). Thus the image of $\mathbf{f}(z)$ is

$$\mathbf{f}(z) = c_0 + c_1 z + c_2 z^2 + \dots \in \mathcal{V}[[z]]. \tag{3.21}$$

The elements $E_i, i = 1, 2, \dots, 2d + 1$ are often called the basis vectors of \mathcal{A} , and their linear combinations are called the vectors of \mathcal{A} . Notice that the F_i are not vectors of \mathcal{A} and so the vectors of \mathcal{A} do not form the space \mathcal{V} . Products of the nonnull vectors of \mathcal{A} are said to form the Lipschitz group [40]. The reversion operator, denoted by a tilde, is defined as the anti-automorphism which reverses the order of the vectors constituting any element of the Lipschitz group and the operation is extended to the whole algebra \mathcal{A} by linearity. For example, if $\alpha, \beta \in \mathbb{R}$ and

$$D = \alpha E_1 + \beta E_4 E_5 E_6,$$

then

$$\tilde{D} = \alpha E_1 + \beta E_6 E_5 E_4.$$

Hence (3.18) and (3.19) imply that

$$\tilde{w} = \sum_{i=1}^d x_i E_i - \sum_{i=1}^d y_i F_i. \tag{3.22}$$

We notice that \tilde{w} corresponds to w^* , the complex conjugate of w , and that

$$\tilde{w}w = \sum_{i=1}^d (x_i^2 + y_i^2)I = \|w\|_2^2 I \tag{3.23}$$

is a real scalar in \mathcal{A} . The linear space of real scalars in \mathcal{A} is defined as $\mathcal{S} := \{\alpha I, \alpha \in \mathbb{R}\}$. Using (3.23) we can form reciprocals, and

$$w^{-1} = \tilde{w}/|w|^2, \tag{3.24}$$

where

$$|w| := \|w\|, \tag{3.25}$$

so that w^{-1} is the image of w^{-1} as defined by (3.5). Thus (3.19) specifies an isomorphism between (i) the space \mathbb{C}^d , having representative element

$$w = x + iy \quad \text{and an inverse} \quad w^{-1} = w^*/\|w\|^2,$$

(ii) the real linear space $\mathcal{V}_{\mathbb{C}}$ with a representative element

$$w = \sum_{i=1}^d x_i E_i + \sum_{i=1}^d y_i F_i \quad \text{and its inverse given by} \quad w^{-1} = \tilde{w}/|w|^2.$$

The isomorphism preserves inverses and linearity with respect to real multipliers, as shown in (3.20). Using this formalism, we proceed to form the polynomial $q_{2j+1}(z)$ analogously to (2.15). The equations for its coefficients are

$$\begin{bmatrix} c_0 & \cdots & c_j \\ \vdots & & \vdots \\ c_j & \cdots & c_{2j} \end{bmatrix} \begin{bmatrix} q_{j+1}^{(2j+1)} \\ \vdots \\ q_1^{(2j+1)} \end{bmatrix} = \begin{bmatrix} -c_{j+1} \\ \vdots \\ -c_{2j+1} \end{bmatrix} \tag{3.26}$$

which represent the accuracy-through-order conditions; we assume that $q_0^{(2j+1)} = q_{2j+1}(0) = I$. In principle, we can eliminate the variables $q_{j+1}^{(2j+1)}, q_j^{(2j+1)}, \dots, q_2^{(2j+1)}$ sequentially, find $q_1^{(2j+1)}$ and then the rest of the variables of (3.26) by back-substitution. However, the resulting $q_i^{(2j+1)}$ turn out to be higher grade quantities in the Clifford algebra, meaning that they involve higher-order outer products of the fundamental vectors. Numerical representation of these quantities uses up computer storage and is undesirable. For practical purposes, we prefer to work with low-grade quantities such as scalars and vectors [42].

The previous remarks reflect the fact that, in general, the product $w_1, w_2, w_3 \notin \mathcal{V}_{\mathbb{C}}$ when $w_1, w_2, w_3 \in \mathcal{V}_{\mathbb{C}}$. However, there is an important exception to this rule, which we formulate as follows [26], see Eqs. (6.3) and (6.4) in [40].

Lemma 3.3. *Let $w, t \in \mathcal{V}_{\mathbb{C}}$ be the images of $w = x + iy, t = u + iv \in \mathbb{C}^d$. Then*

$$(i) \quad t\tilde{w} + w\tilde{t} = 2 \operatorname{Re}(w^H t)I \in \mathcal{S}, \tag{3.27}$$

$$(ii) \quad w\tilde{t}w = 2w \operatorname{Re}(w^H t) - t\|w\|^2 \in \mathcal{V}_{\mathbb{C}}. \tag{3.28}$$

Proof. Using (3.17), (3.18) and (3.22), we have

$$\begin{aligned}
 t\tilde{w} + w\tilde{t} &= \sum_{i=1}^d \sum_{j=1}^d (u_i E_i + v_i F_i)(x_j E_j - y_j F_j) + (x_j E_j + y_j F_j)(u_i E_i - v_i F_i) \\
 &= (\mathbf{u}^T \mathbf{x} + \mathbf{v}^T \mathbf{y})I = 2 \operatorname{Re}(\mathbf{w}^H \mathbf{t})I
 \end{aligned}$$

because, for $i, j = 1, 2, \dots, d$,

$$F_i E_j - E_j F_i = 0, \quad F_i F_j + F_j F_i = -2\delta_{ij}I.$$

For part (ii), we simply note that

$$w\tilde{t}w = w(\tilde{t}w + \tilde{w}t) - w\tilde{w}t. \quad \square$$

We have noted that, as j increases, the coefficients of $q_{2j+1}(z)$ are increasingly difficult to store. Economical approximations to $q_{2j+1}^{(z)}$ are given in [42]. Here we proceed with

$$\begin{bmatrix} c_0 & \cdots & c_{j+1} \\ \vdots & & \vdots \\ c_{j+1} & \cdots & c_{2j+2} \end{bmatrix} \begin{bmatrix} q_{j+1}^{(2j+1)} \\ \vdots \\ q_1^{(2j+1)} \\ I \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ e_{2j+1} \end{bmatrix} \tag{3.29}$$

which are the accuracy-through-order conditions for a right-handed operator Padé approximant (OPA) $p_{2j+1}(z)[q_{2j+1}(z)]^{-1}$ for $f(z)$ arising from

$$f(z)q_{2j+1}(z) = p_{2j+1}(z) + e_{2j+1}z^{2j+2} + O(z^{2j+3}). \tag{3.30}$$

The left-hand side of (3.29) contains a general square Hankel matrix with elements that are operators from \mathcal{C} . A remarkable fact, by no means obvious from (3.29) but proved in the next theorem, is that

$$e_{2j+1} \in \mathcal{C}. \tag{3.31}$$

This result enables us to use OPAs of $f(z)$ without constructing the denominator polynomials. A quantity such as e_{2j+1} in (3.29) is called the left-designant of the operator matrix and it is denoted by

$$e_{2j+1} = \left| \begin{array}{ccc} c_0 & \cdots & c_{j+1} \\ \vdots & & \vdots \\ c_{j+1} & \cdots & c_{2j+2} \end{array} \right|_{\ell}. \tag{3.31b}$$

The subscript ℓ (for left) distinguishes designants from determinants, which are very different constructs. Designants were introduced by Heyting [32] and in this context by Salam [43]. For present purposes, we regard them as being defined by the elimination process following (3.26).

Example 3.4. The denominator of the OPA of type [0/1] is constructed using

$$\begin{bmatrix} c_0 & c_1 \\ c_1 & c_2 \end{bmatrix} \begin{bmatrix} q_1^{(1)} \\ I \end{bmatrix} = \begin{bmatrix} 0 \\ e_1 \end{bmatrix}.$$

We eliminate $q_1^{(1)}$ as described above following (3.26) and find that

$$e_1 = \begin{vmatrix} c_2 & c_1 \\ c_1 & c_0 \end{vmatrix} = c_2 - c_1 c_0^{-1} c_1 \in \text{span}\{c_0, c_1, c_2\}. \tag{3.32}$$

Proceeding with the elimination in (3.29), we obtain

$$\begin{bmatrix} c_2 - c_1 c_0^{-1} c_1 & \cdots & c_{j+2} - c_1 c_0^{-1} c_{j+1} \\ \vdots & & \vdots \\ c_{j+2} - c_{j+1} c_0^{-1} c_1 & \cdots & c_{2j+2} - c_{j+1} c_0^{-1} c_{j+1} \end{bmatrix} \begin{bmatrix} q_{j+2}^{(2j+1)} \\ \vdots \\ q_1^{(2j+1)} \\ I \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ e_{2j+1} \end{bmatrix}. \tag{3.33}$$

Not all the elements of the matrix in (3.33) are vectors. An inductive proof that e_{2j+1} is a vector (at least in the case when the c_j are real vectors and the algebra is a division ring) was given by Salam [43,44] and Roberts [41] using the designant forms of Sylvester’s and Schweins’ identities.

We next construct the numerator and denominator polynomials of the OPAs of $f(z)$ and prove (3.31) using Berlekamp’s method [3], which leads on to the construction of vector Padé approximants.

Definitions. Given the series expansion (3.22) of $f(z)$, numerator and denominator polynomials $A_j(z), B_j(z) \in A[z]$ of degrees ℓ_j, m_j are defined sequentially for $j = 0, 1, 2, \dots$, by

$$A_{j+1}(z) = A_j(z) - zA_{j-1}(z)e_{j-1}^{-1}e_j, \tag{3.34}$$

$$B_{j+1}(z) = B_j(z) - zB_{j-1}(z)e_{j-1}^{-1}e_j \tag{3.35}$$

in terms of the error coefficients e_j and auxiliary polynomials $D_j(z)$ which are defined for $j=0, 1, 2, \dots$ by

$$e_j := [f(z)B_j(z)\tilde{B}_j(z)]_{j+1}, \tag{3.36}$$

$$D_j(z) := \tilde{B}_j(z)B_{j-1}(z)e_{j-1}^{-1}. \tag{3.37}$$

These definitions are initialised with

$$\begin{aligned} A_0(z) &= c_0, & B_0(z) &= I, & e_0 &= c_1, \\ A_{-1}(z) &= 0, & B_{-1}(z) &= I, & e_{-1} &= c_0. \end{aligned} \tag{3.38}$$

Example 3.5.

$$\begin{aligned} A_1(z) &= c_0, & B_1(z) &= I - zc_0^{-1}c_1, & e_1 &= c_2 - c_1c_0^{-1}c_1, \\ D_1(z) &= c_1^{-1} - z\tilde{c}_1\tilde{c}_0^{-1}c_1^{-1}. \end{aligned} \tag{3.39}$$

Lemma 3.6.

$$B_j(0) = I, \quad j = 0, 1, 2, \dots \tag{3.40}$$

Proof. See (3.35) and (3.38). \square

Theorem 3.7. *With the definitions above, for $j = 0, 1, 2, \dots$,*

$$(i) \quad f(z)B_j(z) - A_j(z) = O(z^{j+1}). \tag{3.41}$$

$$(ii) \quad \ell_j := \deg\{A_j(z)\} = [j/2], \quad m_j := \deg\{B_j(z)\} = [(j + 1)/2], \quad \deg\{A_j(z)\tilde{B}_j(z)\} = j. \tag{3.42}$$

$$(iii) \quad B_j(z)\tilde{B}_j(z) = \tilde{B}_j(z)B_j(z) \in \mathcal{S}[z]. \tag{3.43}$$

$$(iv) \quad e_j \in \mathcal{V}_C. \tag{3.44}$$

$$(v) \quad D_j(z), A_j(z)\tilde{B}_j(z) \in \mathcal{V}_C[z]. \tag{3.45}$$

$$(vi) \quad f(z)B_j(z) - A_j(z) = e_j z^{j+1} + O(z^{j+2}). \tag{3.46}$$

Proof. Cases $j=0, 1$ are verified explicitly using (3.38) and (3.39). We make the inductive hypothesis that (i)–(vi) hold for index j as stated, and for index $j - 1$.

Part (i): Using (3.34), (3.35) and the inductive hypothesis (vi),

$$f(z)B_{j+1}(z) - A_{j+1}(z) = f(z)B_j(z) - A_j(z) - z(f(z)B_{j-1}(z) - A_{j-1}(z))e_{j-1}^{-1}e_j = O(z^{j+2}).$$

Part (ii): This follows from (3.34), (3.35) and the inductive hypothesis (ii).

Part (iii): Using (3.27) and (3.35), and hypotheses (iii)–(iv) inductively,

$$\tilde{B}_{j+1}(z)B_{j+1}(z) = \tilde{B}_j(z)B_j(z) + z^2\tilde{B}_{j-1}(z)B_{j-1}(z)|e_j|^2|e_{j-1}|^{-2} - z[D_j(z)e_j + \tilde{e}_j\tilde{D}_j(z)] \in \mathcal{S}[z]$$

and (iii) follows after postmultiplication by $\tilde{B}_{j+1}(z)$ and premultiplication by $[\tilde{B}_{j+1}(z)]^{-1}$, see [37, p. 45].

Part (iv): By definition (3.36),

$$e_{j+1} = \sum_{i=0}^{2m_{j+1}} c_{j+2-i}\beta_i,$$

where each $\beta_i = [B_{j+1}(z)\tilde{B}_{j+1}(z)]_i \in \mathcal{S}$ is real. Hence

$$e_{j+1} \in \mathcal{V}_C.$$

Part (v): From (3.35) and (3.37),

$$D_{j+1}(z) = [\tilde{B}_j(z)B_j(z)]e_j^{-1} - z[\tilde{e}_j\tilde{D}_j(z)e_j^{-1}].$$

Using part (v) inductively, parts (iii), (iv) and Lemma 3.3, it follows that $D_{j+1}(z) \in \mathcal{V}_C[z]$.

Using part (i), (3.40) and the method of proof of part (iv), we have

$$A_{j+1}(z)\tilde{B}_{j+1}(z) = [f(z)B_{j+1}(z)\tilde{B}_{j+1}(z)]_0^{j+1} \in \mathcal{V}_C[z].$$

Part (vi): From part (i), we have

$$f(z)B_{j+1}(z) - A_{j+1}(z) = \gamma_{j+1}z^{j+2} + O(z^{j+3})$$

for some $\gamma_{j+1} \in \mathcal{A}$. Hence,

$$f(z)B_{j+1}(z)\tilde{B}_{j+1}(z) - A_{j+1}(z)\tilde{B}_{j+1}(z) = \gamma_{j+1}z^{j+2}\tilde{B}_{j+1}(z) + O(z^{j+3}).$$

Using (ii) and (3.40), we obtain $\gamma_{j+1} = e_{j+1}$, as required. \square

Corollary. *The designant of a Hankel matrix of real (or complex) vectors is a real (or complex) vector.*

Proof. Any designant of this type is expressed by e_{2j+1} in (3.31b), and (3.44) completes the proof. □

The implications of the previous theorem are extensive. From part (iii) we see that

$$Q_j(z) \cdot I := B_j(z) \tilde{B}_j(z) \tag{3.47}$$

defines a real polynomial $Q_j(z)$. Part (iv) shows that the e_j are images of vectors $e_j \in \mathbb{C}^d$; part (vi) justifies calling them error vectors but they are also closely related to the residuals $\mathbf{b} - A\varepsilon_{2j}^{(0)}$ of Example 3.1. Part (v) shows that $A_j(z)\tilde{B}_j(z)$ is the image of some $\mathbf{P}_j(z) \in \mathbb{C}^d[z]$, so that

$$A_j(z)\tilde{B}_j(z) = \sum_{i=1}^d [\text{Re}\{\mathbf{P}_j\}(z)]_i E_i + \sum_{i=1}^d [\text{Im}\{\mathbf{P}_j\}(z)]_i F_i. \tag{3.48}$$

From (3.17) and (3.18), it follows that

$$\mathbf{P}_j(z) \cdot \mathbf{P}_j^*(z) = Q_j(z) \hat{Q}_j(z), \tag{3.49}$$

where $\hat{Q}_j(z)$ is a real scalar polynomial determined by $\hat{Q}_j(z)I = A_j(z)\tilde{A}_j(z)$. Property (3.49) will later be used to characterise certain VPAs independently of their origins in \mathcal{A} . Operator Padé approximants were introduced in (3.34) and (3.35) so as to satisfy the accuracy-through-order property (3.41) for $f(z)$. To generalise to the full table of approximants, only initialisation (3.38) and the degree specifications (3.42) need to be changed.

For $J > 0$, we use

$$\begin{aligned} A_0^{(J)}(z) &= \sum_{i=0}^J c_i z^i, & B_0^{(J)}(z) &= I, & e_0^{(J)} &= c_{J+1}, \\ A_{-1}^{(J)}(z) &= \sum_{i=0}^{J-1} c_i z^i, & B_{-1}^{(J)}(z) &= I, & e_{-1}^{(J)} &= c_J, \end{aligned} \tag{3.50}$$

$$\ell_j^{(J)} := \text{deg}\{A_j^{(J)}(z)\} = J + [j/2],$$

$$m_j^{(J)} := \text{deg}\{B_j^{(J)}(z)\} = [(j + 1)/2] \tag{3.51}$$

and then (3.38) and (3.42) correspond to the case of $J = 0$.

For $J < 0$, we assume that $c_0 \neq 0$, and define

$$g(z) = [f(z)]^{-1} = \tilde{f}(z)[f(z)\tilde{f}(z)]^{-1} \tag{3.52}$$

corresponding to

$$\mathbf{g}(z) = [\mathbf{f}(z)]^{-1} = \mathbf{f}^*(z)[\mathbf{f}(z) \cdot \mathbf{f}^*(z)]^{-1}. \tag{3.53}$$

(If $c_0 = 0$, we would remove a maximal factor of z^v from $f(z)$ and reformulate the problem.)

Then, for $J < 0$,

$$A_0^{(J)}(z) = I, \quad B_0^{(J)}(z) = \sum_{i=0}^{-J} g_i z^i, \quad e_0^{(J)} = [f(z)B_0^{(J)}(z)]_{1-J},$$

$$A_1^{(J)}(z) = I, \quad B_1^{(J)}(z) = \sum_{i=0}^{1-J} g_i z^i, \quad e_1^{(J)} = [f(z)B_1^{(J)}(z)]_{2-J},$$

$$\ell_j^{(J)} := \deg\{A_j^{(J)}(z)\} = \lfloor j/2 \rfloor,$$

$$m_j^{(J)} := \deg\{B_j^{(J)}(z)\} = \lfloor (j+1)/2 \rfloor - J. \tag{3.54}$$

If an approximant of given type $[\ell/m]$ is required, there are usually two different staircase sequences of the form

$$S^{(J)} = (A_j^{(J)}(z)[B_j^{(J)}(z)]^{-1}, \quad j = 0, 1, 2, \dots) \tag{3.55}$$

which contain the approximant, corresponding to two values of J for which $\ell = \ell_j^{(J)}$ and $m = m_j^{(J)}$. For ease of notation, we use $p^{[\ell/m]}(z) \equiv A_j^{(J)}(z)$ and $q^{[\ell/m]}(z) \equiv B_j^{(J)}(z)$. The construction based on (3.41) is for right-handed OPAs, as in

$$f(z) = p^{[\ell/m]}(z)[q^{[\ell/m]}(z)]^{-1} + O(z^{\ell+m+1}), \tag{3.56}$$

but the construction can easily be adapted to that for left-handed OPAs for which

$$f(z) = [\check{q}^{[\ell/m]}(z)]^{-1} \check{p}^{[\ell/m]}(z) + O(z^{\ell+m+1}). \tag{3.57}$$

Although the left- and right-handed numerator and denominator polynomials usually are different, the actual OPAs of given type are equal:

Theorem 3.8 (Uniqueness). *Left-handed and right-handed OPAs, as specified by (3.56) and (3.57) are identical:*

$$[\ell/m](z) := p^{[\ell/m]}(z)[q^{[\ell/m]}(z)]^{-1} = [\check{q}^{[\ell/m]}(z)]^{-1} \check{p}^{[\ell/m]}(z) \in \mathcal{VC} \tag{3.58}$$

and the OPA of type $[\ell/m]$ for $f(z)$ is unique.

Proof. Cross-multiply (3.58), use (3.56), (3.57) and then (3.40) to establish the formula in (3.58). Uniqueness of $[\ell/m](z)$ follows from this formula too, and its vector character follows from (3.43) and (3.45). \square

The OPAs and the corresponding VPAs satisfy the compass (five-point star) identity amongst approximants of the type shown in the same format as Fig. 3.

Theorem 3.9 (Wynn’s compass identity [57,58]).

$$[N(z) - C(z)]^{-1} + [S(z) - C(z)]^{-1} = [E(z) - C(z)]^{-1} + [W(z) - C(z)]^{-1}. \tag{3.59}$$

Proof. We consider the accuracy-through-order equations for the operators:

$$\check{p}_N(z)q_C(z) - \check{q}_N(z)p_C(z) = z^{\ell+m} \dot{\check{p}}_N \dot{q}_C,$$

$$\check{p}_C(z)q_W(z) - \check{q}_C(z)p_W(z) = z^{\ell+m} \dot{\check{p}}_C \dot{q}_W,$$

$$\check{p}_N(z)q_W(z) - \check{q}_N(z)p_W(z) = z^{\ell+m} \dot{\check{p}}_N \dot{q}_W,$$

where \dot{q}_Ω , \dot{p}_Ω denote the leading coefficients of $p_\Omega(z)$, $q_\Omega(z)$, and care has been taken to respect noncommutativity. Hence

$$\begin{aligned} & [N(z) - C(z)]^{-1} - [W(z) - C(z)]^{-1} \\ &= [N(z) - C(z)]^{-1}(W(z) - N(z))[W(z) - C(z)]^{-1} \\ &= q_C[\check{p}_N q_C - \check{q}_N p_C]^{-1}(\check{q}_N p_W - \check{p}_N q_W)[\check{q}_C p_W - \check{p}_C q_W]^{-1} \check{q}_C \\ &= z^{-\ell-m} q_C(z) \dot{q}_C^{-1} \dot{\check{p}}_C^{-1} \check{q}_C(z). \end{aligned}$$

Similarly, we find that

$$[E(z) - C(z)]^{-1} - [S(z) - C(z)]^{-1} = z^{-\ell-m} q_C(z) \dot{q}_C^{-1} \dot{\check{p}}_C^{-1} \check{q}_C(z)$$

and hence (3.59) is established in its operator form. Complex multipliers are not used in it, and so (3.59) holds as stated. \square

An important consequence of the compass identity is that, with $z = 1$, it becomes equivalent to the vector epsilon algorithm for the construction of $\mathbf{E}(1)$ as we saw in the scalar case. If the elements $s_j \in \mathbf{S}$ have representation (3.14), there exists a scalar polynomial $b(z)$ of degree k such that

$$\mathbf{f}(z) = \mathbf{a}(z)/b(z) \in \mathbb{C}^d[[z]]. \tag{3.60}$$

If the coefficients of $b(z)$ are real, we can uniquely associate an operator $f(z)$ with $\mathbf{f}(z)$ in (3.60), and then the uniqueness theorem implies that

$$\varepsilon_{2k}^{(j)} = f(1) \tag{3.61}$$

and we are apt to say that column $2k$ of the epsilon table is exact in this case. However, Example 3.2 indicates that the condition that $b(z)$ must have real coefficients is not necessary. For greater generality in this respect, generalised inverse, vector-valued Padé approximants (GIPAs) were introduced [22]. The existence of a vector numerator polynomial $\mathbf{P}^{[n/2k]}(z) \in \mathbb{C}^d[z]$ and a real scalar denominator polynomial $Q^{[n/2k]}(z)$ having the following properties is normally established by (3.47) and (3.48):

$$(i) \quad \deg\{\mathbf{P}^{[n/2k]}(z)\} = n, \quad \deg\{Q^{[n/2k]}(z)\} = 2k, \tag{3.62}$$

$$(ii) \quad Q^{[n/2k]}(z) \text{ is a factor of } \mathbf{P}^{[n/2k]}(z) \cdot \mathbf{P}^{[n/2k]*}(z), \tag{3.63}$$

$$(iii) \quad Q^{[n/2k]}(0) = 1, \tag{3.64}$$

$$(iv) \quad \mathbf{f}(z) - \mathbf{P}^{[n/2k]}(z)/Q^{[n/2k]}(z) = O(z^{n+1}), \tag{3.65}$$

where the star in (3.63) denotes the functional complex-conjugate. These axioms suffice to prove the following result.

Theorem 3.10 (Uniqueness [24]). *If the vector-valued Padé approximant*

$$R^{[n/2k]}(z) := P^{[n/2k]}(z)/Q^{[n/2k]}(z) \tag{3.66}$$

of type $[n/2k]$ for $f(z)$ exists, then it is unique.

Proof. Suppose that

$$R(z) = P(z)/Q(z), \quad \hat{R}(z) = \hat{P}(z)/\hat{Q}(z)$$

are two different vector-valued Padé approximants having the same specification as (3.62)–(3.66). Let $Q_{\text{gcd}}(z)$ be the greatest common divisor of $Q(z)$, $\hat{Q}(z)$ and define reduced and coprime polynomials by

$$Q_r(z) = Q(z)/Q_{\text{gcd}}(z), \quad \hat{Q}_r(z) = \hat{Q}(z)/Q_{\text{gcd}}(z).$$

From (3.63) and (3.65) we find that

$$z^{2n+2}Q_r(z)\hat{Q}_r(z) \text{ is a factor of } [P(z)\hat{Q}_r(z) - \hat{P}(z)Q_r(z)] \cdot [P^*(z)\hat{Q}_r(z) - \hat{P}^*(z)Q_r(z)]. \tag{3.67}$$

The left-hand expression of (3.67) is of degree $2n+4k-2 \cdot \text{deg}\{Q_{\text{gcd}}(z)\}+2$. The right-hand expression of (3.67) is of degree $2n+4k-2 \cdot \text{deg}\{Q_{\text{gcd}}(z)\}$. Therefore the right-hand expression of (3.67) is identically zero. \square

By taking $\hat{Q}^{[n/2m]}(z) = b(z)b^*(z)$ and $\hat{P}^{[n/2m]}(z) = a(z)b^*(z)$, the uniqueness theorem shows that the generalised inverse vector-valued Padé approximant constructed using the compass identity yields

$$f(z) = a(z)b^*(z)/b(z)b^*(z)$$

exactly. On putting $z=1$, it follows that the sequence \mathbf{S} , such as the one given by (3.14), is summed exactly by the vector epsilon algorithm in the column of index $2k$. For normal cases, we have now outlined the proof of a principal result [37,2].

Theorem 3.11 (McLeod’s theorem). *Suppose that the vector sequence \mathbf{S} satisfies a nontrivial recursion relation*

$$\sum_{i=0}^k \beta_i s_{i+j} = \left(\sum_{i=0}^k \beta_i \right) s_{\infty}, \quad j = 0, 1, 2, \dots \tag{3.68}$$

with $\beta_i \in \mathbb{C}$. Then the vector epsilon algorithm leads to

$$\varepsilon_{2k}^{(j)} = s_{\infty}, \quad j = 0, 1, 2, \dots \tag{3.69}$$

provided that zero divisors are not encountered in the construction.

The previous theorem is a statement about exact results in the column of index $2k$ in the vector epsilon table. This column corresponds to the row sequence of GIPAs of type $[n/2k]$ for $f(z)$, evaluated at $z=1$. If the given vector sequence \mathbf{S} is nearly, but not exactly, generalized geometric, we model this situation by supposing that its generating function $f(z)$ is analytic in the closed unit disk \bar{D} , except for k poles in $D := \{z: |z| < 1\}$. This hypothesis ensures that $f(z)$ is analytic at $z=1$, and it is sufficiently strong to guarantee convergence of the column of index $2k$ in the vector

epsilon table. There are several convergence theorems of this type [28–30,39]. It is important to note that any row convergence theorem for generalised inverse vector-valued Padé approximants has immediate consequences as a convergence result for a column of the vector epsilon table.

A determinantal formula for $Q^{[n/2k]}(z)$ can be derived [24,25] by exploiting the factorisation property (3.63). The formula is

$$Q^{[n/2k]}(z) = \begin{vmatrix} 0 & M_{01} & M_{02} & \dots & M_{0,2k} \\ M_{10} & 0 & M_{12} & \dots & M_{1,2k} \\ \vdots & \vdots & \vdots & & \vdots \\ M_{2k-1,0} & M_{2k-1,1} & M_{2k-1,2} & \dots & M_{2k-1,2k} \\ z^{2k} & z^{2k-1} & z^{2k-2} & \dots & 1 \end{vmatrix}, \tag{3.70}$$

where the constant entries M_{ij} are those in the first $2k$ rows of an anti-symmetric matrix $M \in \mathbb{R}^{(2k+1) \times (2k+1)}$ defined by

$$M_{ij} = \begin{cases} \sum_{\ell=0}^{j-i-1} \mathbf{c}_{\ell+i+n-2k+1}^H \cdot \mathbf{c}_{j-\ell+n-2k} & \text{for } j > i, \\ -M_{ji} & \text{for } i < j, \\ 0 & \text{for } i = j. \end{cases}$$

As a consequence of the compass identity (Theorem 3.9) and expansion (3.16), we see that entries in the vector epsilon table are given by

$$\varepsilon_{2k}^{(j)} = \mathbf{P}^{[j+2k/2k]}(1) / Q^{[j+2k/2k]}(1), \quad j, k \geq 0,$$

From this result, it readily follows that each entry in the columns of even index in the vector epsilon table is normally given succinctly by a ratio of determinants:

$$\varepsilon_{2k}^{(j)} = \begin{vmatrix} 0 & M_{01} & \dots & M_{0,2k} \\ M_{10} & 0 & \dots & M_{1,2k} \\ \vdots & \vdots & & \vdots \\ M_{2k-1,0} & M_{2k-1,1} & \dots & M_{2k-1,2k} \\ \mathbf{s}_j & \mathbf{s}_{j+1} & \dots & \mathbf{s}_{2k+j} \end{vmatrix} \div \begin{vmatrix} 0 & M_{01} & \dots & M_{0,2k} \\ M_{10} & 0 & \dots & M_{1,2k} \\ \vdots & \vdots & & \vdots \\ M_{2k-1,0} & M_{2k-1,1} & \dots & M_{2k-1,2k} \\ 1 & 1 & \dots & 1 \end{vmatrix}.$$

For computation, it is best to obtain numerical results from (3.4). The coefficients of $Q^{[n/2k]}(z) = \sum_{i=0}^{2k} Q_i^{[n/2k]} z^i$ should be found by solving the homogeneous, anti-symmetric (and therefore consistent) linear system equivalent to (3.70), namely

$$M\mathbf{q} = \mathbf{0},$$

where $\mathbf{q}^T = (Q_{2k-i}^{[n/2k]}, i = 0, 1, \dots, 2k)$.

4. Vector-valued continued fractions and vector orthogonal polynomials

The elements $\varepsilon_{2k}^{(0)}$ lying at the head of each column of even index in the vector epsilon table are values of the convergents of a corresponding continued fraction. In Section 3, we noted that the entries in the vector epsilon table are values of vector Padé approximants of

$$f(z) = c_0 + c_1z + c_2z^2 + \dots \tag{4.1}$$

as defined by (3.16). To obtain the continued fraction corresponding to (4.1), we use Viskovatov’s algorithm, which is an ingenious rule for efficiently performing successive reciprocation and re-expansion of a series [2]. Because algebraic operations are required, we use the image of (4.1) in \mathcal{A} , which is

$$f(z) = c_0 + c_1z + c_2z^2 + \dots \tag{4.2}$$

with $c_i \in \mathcal{V}_C$. Using reciprocation and re-expansion, we find

$$f(z) = \sum_{i=0}^{J-1} c_i z^i + \frac{z^J c_J}{1} - \frac{z\alpha_1^{(J)}}{1} - \frac{z\beta_1^{(J)}}{1} - \frac{z\alpha_2^{(J)}}{1} - \frac{z\beta_2^{(J)}}{1} - \dots \tag{4.3}$$

with $\alpha_i^{(J)}, \beta_i^{(J)} \in \mathcal{A}$ and provided all $\alpha_i^{(J)} \neq 0, \beta_i^{(J)} \neq 0$. By definition, all the inverses implied in (4.3) are to be taken as right-handed inverses. For example, the second convergent of (4.3) is

$$[J + 1/1](z) = \sum_{i=0}^{J-1} c_i z^i + z^J c_J [1 - z\alpha_1^{(J)} [1 - z\beta_1^{(J)}]^{-1}]^{-1}$$

and the corresponding element of the vector epsilon table is

$$\varepsilon_2^{(J)} = [J + 1/1](1),$$

where the type refers to the allowed degrees of the numerator and denominator operator polynomials. The next algorithm is used to construct the elements of (4.3).

Theorem 4.1 (The vector qd algorithm [40]). *With the initialisation*

$$\beta_0^{(J)} = 0, \quad J = 1, 2, 3, \dots, \tag{4.4}$$

$$\alpha_1^{(J)} = c_J^{-1} c_{J+1}, \quad J = 0, 1, 2, \dots, \tag{4.5}$$

the remaining $\alpha_i^{(J)}, \beta_i^{(J)}$ can be constructed using

$$\alpha_m^{(J)} + \beta_m^{(J)} = \alpha_m^{(J+1)} + \beta_{m-1}^{(J+1)}, \tag{4.6}$$

$$\beta_m^{(J)} \alpha_{m+1}^{(J)} = \alpha_m^{(J+1)} \beta_m^{(J+1)} \tag{4.7}$$

for $J = 0, 1, 2, \dots$ and $m = 1, 2, 3, \dots$.

Remark. The elements connected by these rules form lozenges in the $\alpha - \beta$ array, as in Fig. 8. Rule (4.7) requires multiplications which are noncommutative except in the scalar case.

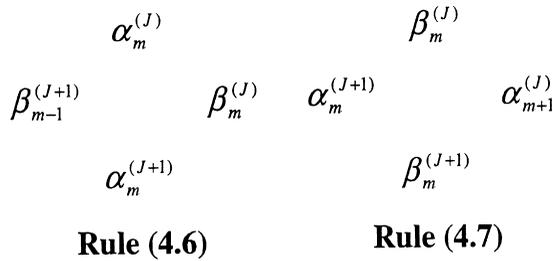


Fig. 8.

Proof. First, the identity

$$C + z\alpha[1 + z\beta D^{-1}]^{-1} = C + z\alpha - z^2\alpha\beta[z\beta + D]^{-1} \tag{4.8}$$

is applied to (4.3) with $\alpha = c_J$, $\beta = -\alpha_1^{(J)}$, then with $\alpha = -\beta_1^{(J)}$, $\beta = -\alpha_2^{(J)}$, etc. We obtain

$$f(z) = \sum_{i=0}^J c_i z^i + \frac{z^{J+1} c_J \alpha_1^{(J)}}{1 - z(\alpha_1^{(J)} + \beta_1^{(J)})} - \frac{z^2 \beta_1^{(J)} \alpha_2^{(J)}}{1 - z(\alpha_2^{(J)} + \beta_2^{(J)})} - \dots \tag{4.9}$$

Secondly, let $J \rightarrow J + 1$ in (4.3), and then apply (4.8) with $\alpha = -\alpha_1^{(J+1)}$, $\beta = -\beta_1^{(J+1)}$, then with $\alpha = -\alpha_2^{(J+1)}$, $\beta = -\beta_2^{(J+1)}$, etc., to obtain

$$f(z) = \sum_{i=0}^J c_i z^i + \frac{z^{J+1} c_{J+1}}{1 - z\alpha_1^{(J+1)}} - \frac{z^2 \alpha_1^{(J+1)} \beta_1^{(J+1)}}{1 - z(\beta_1^{(J+1)} + \alpha_2^{(J+1)})} - \dots \tag{4.10}$$

These expansions (4.9) and (4.10) of $f(z)$ must be identical, and so (4.4)–(4.7) follow by identification of the coefficients. \square

The purpose of this algorithm is the iterative construction of the elements of the C -fraction (4.3) starting from the coefficients c_i of (4.1). However, the elements $\alpha_i^{(J)}, \beta_i^{(J)}$ are not vectors in the algebra. Our next task is to reformulate this algorithm using vector quantities which are amenable for computational purposes.

The recursion for the numerator and denominator polynomials was derived in (3.34) and (3.35) for case of $J = 0$, and the more general sequence of approximants labelled by $J \geq 0$ was introduced in (3.50) and (3.51). For them, the recursions are

$$A_{j+1}^{(J)}(z) = A_j^{(J)}(z) - zA_{j-1}^{(J)}(z)e_{j-1}^{(J)-1}e_j^{(J)}, \tag{4.11}$$

$$B_{j+1}^{(J)}(z) = B_j^{(J)}(z) - zB_{j-1}^{(J)}(z)e_{j-1}^{(J)-1}e_j^{(J)} \tag{4.12}$$

and accuracy-through-order is expressed by

$$f(z)B_j^{(J)}(z) = A_j^{(J)}(z) + e_j^{(J)}z^{j+J+1} + O(z^{j+J+2}) \tag{4.13}$$

for $j=0, 1, 2, \dots$ and $J \geq 0$. Euler’s formula shows that (4.11) and (4.12) are the recursions associated with

$$f(z) = \sum_{i=0}^{J-1} c_i z^i + \frac{c_J z^J}{1} - \frac{e_0^{(J)} z}{1} - \frac{e_0^{(J)-1} e_1^{(J)} z}{1} - \frac{e_1^{(J)-1} e_2^{(J)} z}{1} - \dots \tag{4.14}$$

As was noted for (3.55), the approximant of (operator) type $[J + m/m]$ arising from (4.14) is also a convergent of (4.14) with $J \rightarrow J + 1$. We find that

$$A_{2m}^{(J)}(z)[B_{2m}^{(J)}(z)]^{-1} = [J + m/m](z) = A_{2m-1}^{(J+1)}[B_{2m-1}^{(J+1)}(z)]^{-1} \tag{4.15}$$

and their error coefficients in (4.13) are also the same:

$$e_{2m}^{(J)} = e_{2m-1}^{(J+1)}, \quad m, J = 0, 1, 2, \dots \tag{4.16}$$

These error vectors $e_i^{(J)} \in \mathcal{V}_C$ obey the following identity.

Theorem 4.2 (The cross-rule [27,40,41,46]). *With the partly artificial initialisation*

$$e_{-2}^{(J+1)} = \infty, \quad e_0^{(J)} = c_{J+1} \quad \text{for } J = 0, 1, 2, \dots, \tag{4.17}$$

the error vectors obey the identity

$$e_{i+2}^{(J-1)} = e_i^{(J+1)} + e_i^{(J)}[e_{i-2}^{(J+1)-1} - e_i^{(J-1)-1}]e_i^{(J)} \tag{4.18}$$

for $J \geq 0$ and $i \geq 0$.

Remark. These entries are displayed in Fig. 9 at positions corresponding to their associated approximants (see (4.13)) which satisfy the compass rule.

Proof. We identify the elements of (4.3) and (4.14) and obtain

$$\alpha_{j+1}^{(J)} = e_{2j-1}^{(J-1)} e_{2j}^{(J)}, \quad \beta_{j+1}^{(J)} = e_{2j}^{(J-1)} e_{2j+1}^{(J)}. \tag{4.19}$$

We use (4.16) to standardise on even-valued subscripts for the error vectors in (4.19):

$$\alpha_{j+1}^{(J)} = e_{2j}^{(J-1)-1} e_{2j}^{(J)}, \quad \beta_{j+1}^{(J)} = e_{2j}^{(J-1)} e_{2j+2}^{(J-1)}. \tag{4.20}$$

Substitute (4.20) in (4.6) with $m = j + 1$ and $i = 2j$, giving

$$e_i^{(J-1)-1} e_i^{(J)} + e_i^{(J)-1} e_{i+2}^{(J-1)} = e_i^{(J)-1} e_i^{(J+1)} + e_{i-2}^{(J+1)-1} e_i^{(J)}. \tag{4.21}$$

Result (4.18) follows from (4.21) directly if i is even, but from (4.16) and (4.20) if i is odd. Initialisation (4.17) follows from (3.50). \square

From Fig. 9, we note that the cross-rule can be informally expressed as

$$e_S = e_E + e_C(e_N^{-1} - e_W^{-1})e_C \tag{4.22}$$

where $e_\Omega \in \mathcal{V}_C$ for $\Omega = N, S, E, W$ and C . Because these error vectors are designants (see (3.31b)), Eq. (4.22) is clearly a fundamental compass identity amongst designants.

In fact, this identity has also been established for the leading coefficients \dot{p}_Ω of the numerator polynomials [23]. If we were to use monic normalisation for the denominators

$$\dot{Q}_\Omega(z) = 1, \quad \dot{B}_j^{(J)}(z) = I, \quad \dot{p}_\Omega := \dot{A}_j^{(J)}(z) \tag{4.23}$$

(where the dot denotes that the leading coefficient of the polynomial beneath the dot is required), we would find that

$$\dot{p}_S = \dot{p}_E + \dot{p}_C(\dot{p}_N^{-1} - \dot{p}_W^{-1})\dot{p}_C, \tag{4.24}$$

corresponding to the same compass identity amongst designants.

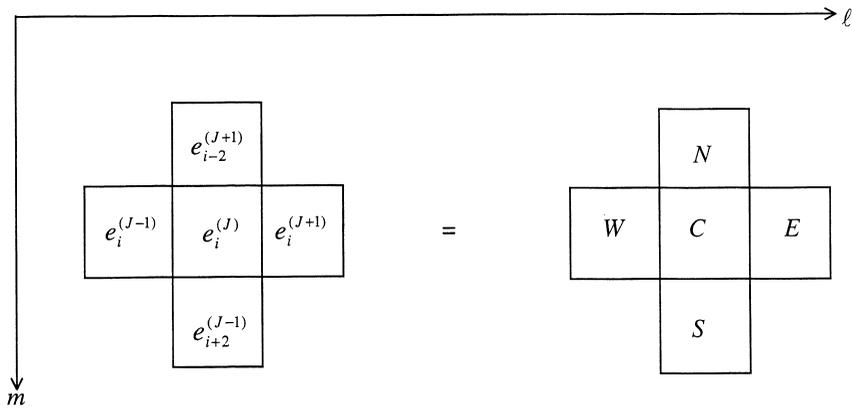


Fig. 9. Position of error vectors obeying the cross-rule.

Reverting to the normalisation of (3.64) with $q_\Omega(0) = I$ and $Q_\Omega(0) = 1$, we note that formula (3.28) is required to convert (4.22) to a usable relation amongst vectors $e_\Omega \in \mathbb{C}^d$. We find that

$$e_S = e_E - |e_C|^2 \left[\frac{e_N}{|e_N|^2} - \frac{e_W}{|e_W|^2} \right] + 2e_C \operatorname{Re} \left[e_C^H \left(\frac{e_N}{|e_N|^2} - \frac{e_W}{|e_W|^2} \right) \right]$$

and this formula is computationally executable.

Implementation of this formula enables the calculation of the vectors e_Ω in \mathbb{C}^d in a rowwise fashion (see Fig. 9). For the case of vector-valued meromorphic functions of the type described following (3.69) it is shown in [40] that asymptotic (i.e., as J tends to infinity) results similar to the scalar case are valid, with an interesting interpretation for the behaviour of the vectors $e_i^{(J)}$ as J tends to infinity. It is also shown in [40] that, as in the scalar case, the above procedure is numerically unstable, while a column-by-column computation retains stability – i.e., (4.22) is used to evaluate e_E . There are also considerations of underflow and overflow which can be dealt with by a mild adaptation of the cross-rule.

Orthogonal polynomials lie at the heart of many approximation methods. In this context, the orthogonal polynomials are operators $\pi_i(\xi) \in \mathcal{A}[\xi]$, and they are defined using the functionals $c\{\cdot\}$ and $\mathbf{c}\{\cdot\}$. These functionals are defined by their action on monomials:

$$c\{\xi^i\} = c_i, \quad \mathbf{c}\{\xi^i\} = \mathbf{c}_i. \tag{4.25}$$

By linearity, we can normally define monic vector orthogonal polynomials by $\pi_0(\xi) = I$ and, for $i = 1, 2, 3, \dots$, by

$$c\{\pi_i(\xi)\xi^j\} = 0, \quad j = 0, 1, \dots, i - 1. \tag{4.26}$$

The connection with the denominator polynomials (3.35) is

Theorem 4.3. For $i = 0, 1, 2, \dots$

$$\pi_i(\xi) = \xi^i B_{2i-1}(\xi^{-1}).$$

Proof. Since $B_{2i-1}(z)$ is an operator polynomial of degree i , so is $\pi_i(\xi)$. Moreover, for $j = 0, 1, \dots, i - 1$,

$$\begin{aligned} c\{\xi^j \pi_i(\xi)\} &= c\{\xi^{i+j} B_{2i-1}(\xi^{-1})\} = \sum_{\ell=0}^i c\{\xi^{i+j-\ell} B_{\ell}^{(2i-1)}\} = \sum_{\ell=0}^i c_{i+j-\ell} B_{\ell}^{(2i-1)} \\ &= [f(z)B_{2i-1}(z)]_{i+j} = 0 \end{aligned}$$

as is required for (4.26). \square

This theorem establishes an equivalence between approximation methods based on vector orthogonal polynomials and those based on vector Padé approximation. To take account of noncommutativity, more care is needed over the issue of linearity with respect to multipliers from \mathcal{A} than is shown in (4.26). Much fuller accounts, using variants of (4.26), are given by Roberts [41] and Salam [44,45].

In this section, we have focussed on the construction and properties of the continued fractions associated with the leading diagonal sequence of vector Padé approximants. When these approximants are evaluated at $z = 1$, they equal $\varepsilon_{2k}^{(0)}$, the entries on the leading diagonal of the vector epsilon table. These entries are our natural first choice for use in the acceleration of convergence of a sequence of vectors.

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Scalar Levin-type sequence transformations

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Abstract

Sequence transformations are important tools for the convergence acceleration of slowly convergent scalar sequences or series and for the summation of divergent series. The basic idea is to construct from a given sequence $\{\{s_n\}\}$ a new sequence $\{\{s'_n\}\} = \mathcal{T}(\{\{s_n\}\})$ where each s'_n depends on a finite number of elements s_{n_1}, \dots, s_{n_m} . Often, the s_n are the partial sums of an infinite series. The aim is to find transformations such that $\{\{s'_n\}\}$ converges faster than (or sums) $\{\{s_n\}\}$. Transformations $\mathcal{T}(\{\{s_n\}\}, \{\{\omega_n\}\})$ that depend not only on the sequence elements or partial sums s_n but also on an auxiliary sequence of the so-called remainder estimates ω_n are of Levin-type if they are linear in the s_n , and nonlinear in the ω_n . Such remainder estimates provide an easy-to-use possibility to use asymptotic information on the problem sequence for the construction of highly efficient sequence transformations. As shown first by Levin, it is possible to obtain such asymptotic information easily for large classes of sequences in such a way that the ω_n are simple functions of a few sequence elements s_n . Then, nonlinear sequence transformations are obtained. Special cases of such Levin-type transformations belong to the most powerful currently known extrapolation methods for scalar sequences and series. Here, we review known Levin-type sequence transformations and put them in a common theoretical framework. It is discussed how such transformations may be constructed by either a model sequence approach or by iteration of simple transformations. As illustration, two new sequence transformations are derived. Common properties and results on convergence acceleration and stability are given. For important special cases, extensions of the general results are presented. Also, guidelines for the application of Levin-type sequence transformations are discussed, and a few numerical examples are given. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

In applied mathematics and the numerate sciences, extrapolation methods are often used for the convergence acceleration of slowly convergent sequences or series and for the summation of divergent series. For an introduction to such methods, and also further information that cannot be covered here, see the books of Brezinski and Redivo Zaglia [14] and Wimp [102] and the work of Weniger [84,88] and Homeier [40], but also the books of Baker [3], Baker and Graves-Morris [5], Brezinski [7,8,10–12], Graves-Morris [24,25], Graves-Morris, Saff and Varga [26], Khovanskii [52], Lorentzen and Waadeland [56], Nikishin and Sorokin [62], Petrushev and Popov [66], Ross [67], Saff and Varga [68], Wall [83], Werner and Buenger [101] and Wuytack [103].

For the discussion of extrapolation methods, one considers a sequence $\{\{s_n\}\} = \{\{s_0, s_1, \dots\}\}$ with elements s_n or the terms $a_n = s_n - s_{n-1}$ of a series $\sum_{j=0}^{\infty} a_j$ with partial sums $s_n = \sum_{j=0}^n a_j$ for large n . A common approach is to rewrite s_n as

$$s_n = s + R_n, \quad (1)$$

where s is the limit (or antilimit in the case of divergence) and R_n is the remainder or tail. The aim then is to find a new sequence $\{\{s'_n\}\}$ such that

$$s'_n = s + R'_n, \quad R'_n/R_n \rightarrow 0 \text{ for } n \rightarrow \infty. \quad (2)$$

Thus, the sequence $\{\{s'_n\}\}$ converges faster to the limit s (or diverges less violently) than $\{\{s_n\}\}$.

To find the sequence $\{\{s'_n\}\}$, i.e., to construct a sequence transformation $\{\{s'_n\}\} = \mathcal{T}(\{\{s_n\}\})$, one needs asymptotic information about the s_n or the terms a_n for large n , and hence about the R_n . This information then allows to eliminate the remainder at least asymptotically, for instance by subtracting the dominant part of the remainder. Either such information is obtained by a careful mathematical analysis of the behavior of the s_n and/or a_n , or it has to be extracted numerically from the values of a finite number of the s_n and/or a_n by some method that ideally can be proven to work for a large class of problems.

Suppose that one knows quantities ω_n such that $R_n/\omega_n = O(1)$ for $n \rightarrow \infty$, for instance

$$\lim_{n \rightarrow \infty} R_n/\omega_n = c \neq 0, \quad (3)$$

where c is a constant. Such quantities are called remainder estimates. Quite often, such remainder estimates can be found with relatively low effort but the exact value of c is often quite hard to calculate. Then, it is rather natural to rewrite the rest as $R_n = \omega_n \mu_n$ where $\mu_n \rightarrow c$. The problem is how to describe or model the μ_n . Suppose that one has a system of known functions $\psi_j(n)$ such that $\psi_0(n) = 1$ and $\psi_{j+1} = o(\psi_j(n))$ for $j \in \mathbb{N}_0$. An example of such a system is $\psi_j(n) = (n + \beta)^{-j}$ for some $\beta \in \mathbb{R}_+$. Then, one may model μ_n as a linear combination of the $\psi_j(n)$ according to

$$\mu_n \sim \sum_{j=0}^{\infty} c_j \psi_j(n) \quad \text{for } n \rightarrow \infty, \quad (4)$$

whence the problem sequence is modelled according to

$$s_n \sim s + \omega_n \sum_{j=0}^{\infty} c_j \psi_j(n). \quad (5)$$

The idea now is to eliminate the leading terms of the remainder with the unknown constants c_j up to $j = k - 1$, say. Thus, one uses a model sequence with elements

$$\sigma_m = \sigma + \omega_m \sum_{j=0}^{k-1} c_j \psi_j(m), \quad m \in \mathbb{N}_0 \quad (6)$$

and calculates σ exactly by solving the system of $k + 1$ equations resulting for $m = n, n + 1, \dots, n + k$ for the unknowns σ and c_j , $j = 0, \dots, k - 1$. The solution for σ is a ratio of determinants (see below) and may be denoted symbolically as

$$\sigma = T(\sigma_n, \dots, \sigma_{n+k}; \omega_n, \dots, \omega_{n+k}; \psi_j(n), \dots, \psi_j(n + k)). \quad (7)$$

The resulting sequence transformation is

$$\mathcal{T}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \{\{\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\})\}\} \quad (8)$$

with

$$\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = T(s_n, \dots, s_{n+k}; \omega_n, \dots, \omega_{n+k}; \psi_j(n), \dots, \psi_j(n + k)). \quad (9)$$

It eliminates the leading terms of the asymptotic expansion (5). The model sequences (6) are in the kernel of the sequence transformation \mathcal{T} , defined as the set of all sequences such that \mathcal{T} reproduces their (anti)limit exactly.

A somewhat more general approach is based on model sequences of the form

$$\sigma_n = \sigma + \sum_{j=1}^k c_j g_j(n), \quad n \in \mathbb{N}_0, \quad k \in \mathbb{N}. \quad (10)$$

Virtually all known sequence transformations can be derived using such model sequences. This leads to the **E** algorithm as described below in Section 3.1. Also, some further important examples of sequence transformations are described in Section 3.

However, the introduction of remainder estimates proved to be an important theoretical step since it allows to make use of asymptotic information of the remainder easily. The most prominent of the resulting sequence transformations $\mathcal{T}(\{\{s_n\}\}, \{\{\omega_n\}\})$ is the Levin transformation [53] that corresponds to the asymptotic system of functions given by $\psi_j(n) = (n + \beta)^{-j}$, and thus, to Poincaré-type expansions of the μ_n . But also other systems are of importance, like $\psi_j(n) = 1/(n + \beta)_j$ leading to factorial series, or $\psi_j(n) = t_n^j$ corresponding to Taylor expansions of t -dependent functions at the abscissae t_n that tend to zero for large n . The question which asymptotic system is best, cannot be decided generally. The answer to this question depends on the extrapolation problem. To obtain efficient extrapolation procedures for large classes of problems requires to use various asymptotic systems, and thus, a larger number of different sequence transformations. Also, different choices of ω_n lead to different variants of such transformations. Levin [53] has pioneered this question and introduced three variants that are both simple and rather successful for large classes of problems. These variants and some further ones will be discussed. The question which variant is best, also

cannot be decided generally. There are, however, a number of results that favor certain variants for certain problems. For example, for Stieltjes series, the choice $\omega_n = a_{n+1}$ can be theoretically justified (see Appendix A).

Thus, we will focus on sequence transformations that involve an auxiliary sequence $\{\{\omega_n\}\}$. To be more specific, we consider transformations of the form $\mathcal{T}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \{\{\mathcal{T}_n^{(k)}\}\}$ with

$$\mathcal{T}_n^{(k)} = \frac{\sum_{j=0}^k \lambda_{n,j}^{(k)} s_{n+j} / \omega_{n+j}}{\sum_{j=0}^k \lambda_{n,j}^{(k)} / \omega_{n+j}}. \quad (11)$$

This will be called a Levin-type transformations. The known sequence transformations that involve remainder estimates, for instance the \mathcal{C} , \mathcal{S} , and \mathcal{M} transformations of Weniger [84], the W algorithm of Sidi [73], and the \mathcal{J} transformation of Homeier with its many special cases like the important ${}_p\mathbf{J}$ transformations [35,36,38–40,46], are all of this type. Interestingly, also the \mathcal{H} , \mathcal{I} , and \mathcal{K} transformations of Homeier [34,35,37,40–44] for the extrapolation of orthogonal expansions are of this type although the ω_n in some sense cease to be remainder estimates as defined in Eq. (3).

The Levin transformation was also generalized in a different way by Levin and Sidi [54] who introduced the $d^{(m)}$ transformations. This is an important class of transformations that would deserve a thorough review itself. This, however, is outside the scope of the present review. We collect some important facts regarding this class of transformations in Section 3.2.

Levin-type transformations as defined in Eq. (11) have been used for the solution of a large variety of problems. For instance, Levin-type sequence transformations have been applied for the convergence acceleration of infinite series representations of molecular integrals [28,29,33,65,82,98–100], for the calculation of the lineshape of spectral holes [49], for the extrapolation of cluster- and crystal-orbital calculations of one-dimensional polymer chains to infinite chain length [16,88,97], for the calculation of special functions [28,40,82,88,89,94,100], for the summation of divergent and acceleration of convergent quantum mechanical perturbation series [17,18,27,85,90–93,95,96], for the evaluation of semiinfinite integrals with oscillating integrands and Sommerfeld integral tails [60,61,75,81], and for the convergence acceleration of multipolar and orthogonal expansions and Fourier series [34,35,37,40–45,63,77,80]. This list is clearly not complete but sufficient to demonstrate the possibility of successful application of these transformations.

The outline of this survey is as follows: After listing some definitions and notations, we discuss some basic sequence transformations in order to provide some background information. Then, special definitions relevant for Levin-type sequence transformations are given, including variants obtained by choosing specific remainder estimates ω_n . After this, important examples of Levin-type sequence transformations are introduced. In Section 5, we will discuss approaches for the construction of Levin-type sequence transformations, including model sequences, kernels and annihilation operators, and also the concept of hierarchical consistency. In Section 6, we derive basic properties, those of limiting transformations and discuss the application to power series. In Section 7, results on convergence acceleration are presented, while in Section 8, results on the numerical stability of the transformations are provided. Finally, we discuss guidelines for the application of the transformations and some numerical examples in Section 9.

2. Definitions and notations

2.1. General definitions

2.1.1. Sets

Natural numbers:

$$\mathbb{N} = \{1, 2, 3, \dots\}, \quad \mathbb{N}_0 = \mathbb{N} \cup \{0\}. \quad (12)$$

Integer numbers:

$$\mathbb{Z} = \mathbb{N} \cup \{0, -1, -2, -3, \dots\}. \quad (13)$$

Real numbers and vectors:

$$\begin{aligned} \mathbb{R} &= \{x : x \text{ real}\}, \\ \mathbb{R}_+ &= \{x \in \mathbb{R} : x > 0\} \\ \mathbb{R}^n &= \{(x_1, \dots, x_n) \mid x_j \in \mathbb{R}, j = 1, \dots, n\}. \end{aligned} \quad (14)$$

Complex numbers:

$$\begin{aligned} \mathbb{C} &= \{z = x + iy : x \in \mathbb{R}, y \in \mathbb{R}, i^2 = -1\}, \\ \mathbb{C}^n &= \{(z_1, \dots, z_n) \mid z_j \in \mathbb{C}, j = 1, \dots, n\}. \end{aligned} \quad (15)$$

For $z = x + iy$, real and imaginary parts are denoted as $x = \Re(z)$, $y = \Im(z)$. We use \mathbb{K} to denote \mathbb{R} or \mathbb{C} .

Vectors with nonvanishing components:

$$\mathbb{F}^n = \{(z_1, \dots, z_n) \mid z_j \in \mathbb{C}, z_j \neq 0, j = 1, \dots, n\}. \quad (16)$$

Polynomials:

$$\mathbb{P}^k = \left\{ P : z \mapsto \sum_{j=0}^k c_j z^j \mid z \in \mathbb{C}, (c_0, \dots, c_k) \in \mathbb{K}^{k+1} \right\}. \quad (17)$$

Sequences:

$$\mathbb{S}^{\mathbb{K}} = \{ \{ \{ s_0, s_1, \dots, s_n, \dots \} \} \mid s_n \in \mathbb{K}, n \in \mathbb{N}_0 \}. \quad (18)$$

Sequences with nonvanishing terms:

$$\mathbb{O}^{\mathbb{K}} = \{ \{ \{ s_0, s_1, \dots, s_n, \dots \} \} \mid s_n \neq 0, s_n \in \mathbb{K}, n \in \mathbb{N}_0 \}. \quad (19)$$

2.1.2. Special functions and symbols

Gamma function [58, p. 1]:

$$\Gamma(z) = \int_0^\infty t^{z-1} \exp(-t) dt \quad (z \in \mathbb{R}_+). \quad (20)$$

Factorial:

$$n! = \Gamma(n+1) = \prod_{j=1}^n j. \quad (21)$$

Pochhammer symbol [58, p. 2]:

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} = \prod_{j=1}^n (a+j-1). \quad (22)$$

Binomial coefficients [1, p. 256, Eq. (6.1.21)]:

$$\binom{z}{w} = \frac{\Gamma(z+1)}{\Gamma(w+1)\Gamma(z-w+1)}. \quad (23)$$

Entier function:

$$\llbracket x \rrbracket = \max\{j \in \mathbb{Z}: j \leq x, x \in \mathbb{R}\}. \quad (24)$$

2.2. Sequences, series and operators

2.2.1. Sequences and series

For Stieltjes series see Appendix A.

Scalar sequences with elements s_n , tail R_n , and limit s :

$$\{\{s_n\}\} = \{\{s_n\}\}_{n=0}^\infty = \{\{s_0, s_1, s_2, \dots\}\} \in \mathbb{S}^{\mathbb{K}}, \quad R_n = s_n - s, \quad \lim_{n \rightarrow \infty} s_n = s. \quad (25)$$

If the sequence is not convergent but summable to s , s is called the antilimit. The n th element s_n of a sequence $\sigma = \{\{s_n\}\} \in \mathbb{S}^{\mathbb{K}}$ is also denoted by $\langle \sigma \rangle_n$. A sequence is called a *constant sequence*, if all elements are constant, i.e., if there is a $c \in \mathbb{K}$ such that $s_n = c$ for all $n \in \mathbb{N}_0$, in which case it is denoted by $\{\{c\}\}$. The constant sequence $\{\{0\}\}$ is called the *zero sequence*.

Scalar series with terms $a_j \in \mathbb{K}$, partial sums s_n , tail R_n , and limit/antilimit s :

$$s = \sum_{j=0}^\infty a_j, \quad s_n = \sum_{j=0}^n a_j, \quad R_n = - \sum_{j=n+1}^\infty a_j = s_n - s. \quad (26)$$

We say that \hat{a}_n are Kummer-related to the a_n with limit or antilimit \hat{s} if $\hat{a}_n = \Delta \hat{s}_{n-1}$ satisfy $a_n \sim \hat{a}_n$ for $n \rightarrow \infty$ and \hat{s} is the limit (or antilimit) of $\hat{s}_n = \sum_{j=0}^n \hat{a}_j$.

Scalar power series in $z \in \mathbb{C}$ with coefficients $c_j \in \mathbb{K}$, partial sums $f_n(z)$, tail $R_n(z)$, and limit/antilimit $f(z)$:

$$f(z) = \sum_{j=0}^\infty c_j z^j, \quad f_n(z) = \sum_{j=0}^n c_j z^j, \quad R_n(z) = \sum_{j=n+1}^\infty c_j z^j = f(z) - f_n(z). \quad (27)$$

2.2.2. Types of convergence

Sequences $\{\{s_n\}\}$ satisfying the equation

$$\lim_{n \rightarrow \infty} (s_{n+1} - s)/(s_n - s) = \rho \quad (28)$$

are called *linearly convergent* if $0 < |\rho| < 1$, *logarithmically convergent* for $\rho = 1$ and *hyperlinearly convergent* for $\rho = 0$. For $|\rho| > 1$, the sequence diverges.

A sequence $\{\{u_n\}\}$ accelerates a sequence $\{\{v_n\}\}$ to s if

$$\lim_{n \rightarrow \infty} (u_n - s)/(v_n - s) = 0. \quad (29)$$

If $\{\{v_n\}\}$ converges to s then we also say that $\{\{u_n\}\}$ converges faster than $\{\{v_n\}\}$.

A sequence $\{\{u_n\}\}$ accelerates a sequence $\{\{v_n\}\}$ to s with order $\alpha > 0$ if

$$(u_n - s)/(v_n - s) = O(n^{-\alpha}). \tag{30}$$

If $\{\{v_n\}\}$ converges to s then we also say that $\{\{u_n\}\}$ converges faster than $\{\{v_n\}\}$ with order α .

2.2.3. Operators

Annihilation operator: An operator $\mathcal{A}: \mathbb{S}^{\mathbb{K}} \rightarrow \mathbb{K}$ is called an annihilation operator for a given sequence $\{\{\tau_n\}\}$ if it satisfies

$$\begin{aligned} \mathcal{A}(\{\{s_n + zt_n\}\}) &= \mathcal{A}(\{\{s_n\}\}) + z\mathcal{A}(\{\{t_n\}\}) \quad \text{for all } \{\{s_n\}\} \in \mathbb{S}^{\mathbb{K}}, \{\{t_n\}\} \in \mathbb{S}^{\mathbb{K}}, z \in \mathbb{K}, \\ \mathcal{A}(\{\{\tau_n\}\}) &= 0. \end{aligned} \tag{31}$$

Forward difference operator.

$$\begin{aligned} \Delta_m g(m) &= g(m + 1) - g(m), \quad \Delta_m g_m = g_{m+1} - g_m, \\ \Delta_m^k &= \Delta_m \Delta_m^{k-1}, \\ \Delta &= \Delta_n, \\ \Delta^k g_n &= \sum_{j=0}^k (-1)^{k-j} \binom{k}{j} g_{n+j}. \end{aligned} \tag{32}$$

Generalized difference operator $\nabla_n^{(k)}$ for given quantities $\delta_n^{(k)} \neq 0$:

$$\nabla_n^{(k)} = (\delta_n^{(k)})^{-1} \Delta. \tag{33}$$

Generalized difference operator $\tilde{\nabla}_n^{(k)}$ for given quantities $\zeta_n^{(k)} \neq 0$:

$$\tilde{\nabla}_n^{(k)} = (\zeta_n^{(k)})^{-1} \Delta^2. \tag{34}$$

Generalized difference operator $\nabla_n^{(k)}[\alpha]$ for given quantities $\Delta_n^{(k)} \neq 0$:

$$\nabla_n^{(k)}[\alpha] f_n = (\Delta_n^{(k)})^{-1} (f_{n+2} - 2 \cos \alpha f_{n+1} + f_n). \tag{35}$$

Generalized difference operator $\partial_n^{(k)}[\zeta]$ for given quantities $\tilde{\Delta}_n^{(k)} \neq 0$:

$$\partial_n^{(k)}[\zeta] f_n = (\tilde{\Delta}_n^{(k)})^{-1} (\zeta_{n+k}^{(2)} f_{n+2} + \zeta_{n+k}^{(1)} f_{n+1} + \zeta_{n+k}^{(0)} f_n). \tag{36}$$

Weighted difference operators for given $P^{(k-1)} \in \mathbb{P}^{k-1}$:

$$\mathcal{W}_n^{(k)} = \mathcal{W}_n^{(k)}[P^{(k-1)}] = \Delta^{(k)} P^{(k-1)}(n). \tag{37}$$

Polynomial operators \mathcal{P} for given $P^{(k)} \in \mathbb{P}^{(k)}$: Let $P^{(k)}(x) = \sum_{j=0}^k p_j^{(k)} x^j$. Then put

$$\mathcal{P}[P^{(k)}] g_n = \sum_{j=0}^k p_j^{(k)} g_{n+j}. \tag{38}$$

Divided difference operator. For given $\{\{x_n\}\}$ and $k, n \in \mathbb{N}_0$, put

$$\square_n^{(k)}[\{\{x_n\}\}](f(x)) = \square_n^{(k)}(f(x)) = f[x_n, \dots, x_{n+k}] = \sum_{j=0}^k f(x_{n+j}) \prod_{\substack{i=0 \\ i \neq j}}^k \frac{1}{x_{n+j} - x_{n+i}},$$

$$\square_n^{(k)}[\{\{x_n\}\}]g_n = \square_n^{(k)}g_n = \sum_{j=0}^k g_{n+j} \prod_{\substack{i=0 \\ i \neq j}}^k \frac{1}{x_{n+j} - x_{n+i}}. \quad (39)$$

3. Some basic sequence transformations

3.1. E Algorithm

Putting for sequences $\{\{y_n\}\}$ and $\{\{g_j(n)\}\}$, $j = 1, \dots, k$

$$E_n^{(k)}[\{\{y_n\}\}; \{\{g_j(n)\}\}] = \begin{vmatrix} y_n & \cdots & y_{n+k} \\ g_1(n) & \cdots & g_1(n+k) \\ \vdots & \ddots & \vdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}, \quad (40)$$

one may define the sequence transformation

$$\mathbf{E}_n^{(k)}(\{\{s_n\}\}) = \frac{E_n^{(k)}[\{\{s_n\}\}; \{\{g_j(n)\}\}]}{E_n^{(k)}[\{\{1\}\}; \{\{g_j(n)\}\}]}. \quad (41)$$

As is plain using Cramer's rule, we have $\mathbf{E}_n^{(k)}(\{\{s_n\}\}) = \sigma$ if the s_n satisfy Eq. (10). Thus, the sequence transformation yields the limit σ exactly for model sequences (10).

The sequence transformation \mathbf{E} is known as the \mathbf{E} algorithm or also as Brezinski–Håvie–Protocol [102, Section 10] after two of its main investigators, Håvie [32] and Brezinski [9]. A good introduction to this transformation is also given in the book of Brezinski and Redivo Zaglia [14, Section 2.1], cf. also Ref. [15].

Numerically, the computation of the $\mathbf{E}_n^{(k)}(\{\{s_n\}\})$ can be performed recursively using either the algorithm of Brezinski [14, p. 58f]

$$\begin{aligned} \mathbf{E}_n^{(0)}(\{\{s_n\}\}) &= s_n, & g_{0,i}^{(n)} &= g_i(n), & n &\in \mathbb{N}_0, & i &\in \mathbb{N}, \\ \mathbf{E}_n^{(k)}(\{\{s_n\}\}) &= \mathbf{E}_n^{(k-1)}(\{\{s_n\}\}) - \frac{\mathbf{E}_{(n+1)}^{(k-1)}(\{\{s_n\}\}) - \mathbf{E}_n^{(k-1)}(\{\{s_n\}\})}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}} g_{k-1,k}^{(n)}, \\ g_{k,i}^{(n)} &= g_{k-1,i}^{(n)} - \frac{g_{k-1,i}^{(n+1)} - g_{k-1,i}^{(n)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}} g_{k-1,1,k}^{(n)}, & i &= k+1, k+2, \dots \end{aligned} \quad (42)$$

or the algorithm of Ford and Sidi [22] that requires additionally the quantities $g_{k+1}(n+j)$, $j=0, \dots, k$ for the computation of $\mathbf{E}_n^{(k)}(\{\{s_n\}\})$. The algorithm of Ford and Sidi involves the quantities

$$\Psi_{k,n}(u) = \frac{E_n^{(k)}[\{\{u_n\}\}; \{\{g_j(n)\}\}]}{E_n^{(k)}[\{\{g_{k+1}(n)\}\}; \{\{g_j(n)\}\}]} \quad (43)$$

for any sequence $\{\{u_0, u_1, \dots\}\}$, where the $g_i(n)$ are not changed even if they depend on the u_n and the u_n are changed. Then we have

$$\mathbf{E}_n^{(k)}(\{\{s_n\}\}) = \frac{\Psi_k^{(n)}(s)}{\Psi_k^{(n)}(1)} \quad (44)$$

and the Ψ are calculated recursively via

$$\Psi_{k,n}(u) = \frac{\Psi_{k-1,n+1}(u) - \Psi_{k-1,n}(u)}{\Psi_{k-1,n+1}(g_{k+1}) - \Psi_{k-1,n}(g_{k+1})}. \tag{45}$$

Of course, for $g_j(n) = \omega_n \psi_{j-1}(n)$, i.e., in the context of sequences modelled via expansion (5), the E algorithm may be used to obtain an explicit representation for any Levin-type sequence transformation of the form (cf. Eq. (9))

$$\mathcal{F}_n^{(k)} = T(s_n, \dots, s_{n+k}; \omega_n, \dots, \omega_{n+k}; \psi_j(n), \dots, \psi_j(n+k)) \tag{46}$$

as ratio of two determinants

$$\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{E_n^{(k)}[\{\{s_n/\omega_n\}\}; \{\{\psi_{j-1}(n)\}\}]}{E_n^{(k)}[\{\{1/\omega_n\}\}; \{\{\psi_{j-1}(n)\}\}]} \tag{47}$$

This follows from the identity [14]

$$\frac{E_n^{(k)}[\{\{s_n\}\}; \{\{\omega_n \psi_{j-1}(n)\}\}]}{E_n^{(k)}[\{\{1\}\}; \{\{\omega_n \psi_{j-1}(n)\}\}]} = \frac{E_n^{(k)}[\{\{s_n/\omega_n\}\}; \{\{\psi_{j-1}(n)\}\}]}{E_n^{(k)}[\{\{1/\omega_n\}\}; \{\{\psi_{j-1}(n)\}\}]} \tag{48}$$

that is an easy consequence of usual algebraic manipulations of determinants.

3.2. The $d^{(m)}$ transformations

As noted in the introduction, the $d^{(m)}$ transformations were introduced by Levin and Sidi [54] as a generalization of the u variant of the Levin transformation [53]. We describe a slightly modified variant of the $d^{(m)}$ transformations [77]:

Let $s_r, r = 0, 1, \dots$ be a real or complex sequence with limit or antilimit s and terms $a_0 = s_0$ and $a_r = s_r - s_{r-1}, r = 1, 2, \dots$ such that $s_r = \sum_{j=0}^r a_j, r = 0, 1, \dots$. For given $m \in \mathbb{N}$ and $\xi_l \in \mathbb{N}_0$ with $l \in \mathbb{N}_0$ and $0 \leq \xi_0 < \xi_1 < \xi_2 < \dots$ and $v = (n_1, \dots, n_m)$ with $n_j \in \mathbb{N}_0$ the $d^{(m)}$ transformation yields a table of approximations $s_v^{(m,j)}$ for the (anti-)limit s as solution of the linear system of equations

$$s_{\xi_l} = s_v^{(m,j)} + \sum_{k=1}^m (\xi_l + \alpha)^k [\Delta^{k-1} a_{\xi_l}] \sum_{i=0}^{n_k} \frac{\bar{\beta}_{ki}}{(\xi_l + \alpha)^i}, \quad j \leq l \leq j + N \tag{49}$$

with $\alpha > 0, N = \sum_{k=1}^m n_k$ and the $N+1$ unknowns $s_v^{(m,j)}$ and $\bar{\beta}_{ki}$. The $[\Delta^k a_j]$ are defined via $[\Delta^0 a_j] = a_j$ and $[\Delta^k a_j] = [\Delta^{k-1} a_{j+1}] - [\Delta^{k-1} a_j], k = 1, 2, \dots$. In most cases, all n_k are chosen equal and one puts $v = (n, n, \dots, n)$. Apart from the value of α , only the input of m and of ξ_l is required from the user. As transformed sequence, often one chooses the elements $s_{(n, \dots, n)}^{(m,0)}$ for $n = 0, 1, \dots$. The u variant of the Levin transformation is obtained for $m = 1, \alpha = \beta$ and $\xi_l = l$. The definition above differs slightly from the original one [54] and was given in Ref. [22] with $\alpha = 1$.

Ford and Sidi have shown, how these transformations can be calculated recursively with the $\mathbf{W}^{(m)}$ algorithms [22]. The $d^{(m)}$ transformations are the best known special cases of the *generalised Richardson Extrapolation process* (GREP) as defined by Sidi [72,73,78].

The $d^{(m)}$ transformations are derived by asymptotic analysis of the remainders $s_r - s$ for $r \rightarrow \infty$ for the family $\tilde{B}^{(m)}$ of sequences $\{\{a_r\}\}$ as defined in Ref. [54]. For such sequences, the a_r satisfy a difference equation of order m of the form

$$a_r = \sum_{k=1}^m p_k(r) \Delta^k a_r. \tag{50}$$

The $p_k(r)$ satisfy the asymptotic relation

$$p_k(r) \sim r^{i_k} \sum_{\ell=0}^{\infty} \frac{P_{k\ell}}{r^\ell} \quad \text{for } r \rightarrow \infty. \tag{51}$$

The i_k are integers satisfying $i_k \leq k$ for $k = 1, \dots, m$. This family of sequences is very large. But still, Levin and Sidi could prove [54, Theorem 2] that under mild additional assumptions, the remainders for such sequences satisfy

$$s_r - s \sim \sum_{k=1}^m r^{j_k} (\Delta^{k-1} a_r) \sum_{\ell=0}^{\infty} \frac{\beta_{k\ell}}{r^\ell} \quad \text{for } r \rightarrow \infty. \tag{52}$$

The j_k are integers satisfying $j_k \leq k$ for $k = 1, \dots, m$. A corresponding result for $m = 1$ was proven by Sidi [71, Theorem 6.1].

System (49) now is obtained by truncation of the expansions at $\ell = n$, evaluation at $r = \xi_l$, and some further obvious substitutions.

The introduction of suitable ξ_l was shown to improve the accuracy and stability in difficult situations considerably [77].

3.3. Shanks transformation and epsilon algorithm

An important special case of the **E** algorithm is the choice $g_j(n) = \Delta_{s_{n+j-1}}$ leading to the Shanks transformation [70]

$$e_k(s_n) = \frac{E_n^{(k)}[\{\{s_n\}\}; \{\{\Delta_{s_{n+j-1}}\}\}]}{E_n^{(k)}[\{\{1\}\}; \{\{\Delta_{s_{n+j-1}}\}\}]} \tag{53}$$

Instead of using one of the recursive schemes for the **E** algorithms, the Shanks transformation may be implemented using the epsilon algorithm [104] that is defined by the recursive scheme

$$\begin{aligned} \varepsilon_{-1}^{(n)} &= 0, & \varepsilon_0^{(n)} &= s_n, \\ \varepsilon_{k+1}^{(n)} &= \varepsilon_{k-1}^{(n+1)} + 1/[\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}]. \end{aligned} \tag{54}$$

The relations

$$\varepsilon_{2k}^{(n)} = e_k(s_n), \quad \varepsilon_{2k+1}^{(n)} = 1/e_k(\Delta s_n) \tag{55}$$

hold and show that the elements $\varepsilon_{2k+1}^{(n)}$ are only auxiliary quantities.

The kernel of the Shanks transformation e_k is given by sequences of the form

$$s_n = s + \sum_{j=0}^{k-1} c_j \Delta s_{n+j}. \tag{56}$$

See also [14, Theorem 2.18].

Additionally, one can use the Shanks transformation – and hence the epsilon algorithm – to compute the upper-half of the Padé table according to [70,104]

$$e_k(f_n(z)) = [n + k/k]_r(z) \quad (k \geq 0, n \geq 0), \tag{57}$$

where

$$f_n(z) = \sum_{j=0}^n c_j z^j \tag{58}$$

are the partial sums of a power series of a function $f(z)$. Padé approximants of $f(z)$ are rational functions in z given as ratio of two polynomials $p_\ell \in \mathbb{P}^{(\ell)}$ and $q_m \in \mathbb{P}^{(m)}$ according to

$$[\ell/m]_f(z) = p_\ell(z)/q_m(z), \tag{59}$$

where the Taylor series of f and $[\ell/m]_f$ are identical to the highest possible power of z , i.e.,

$$f(z) - p_\ell(z)/q_m(z) = O(z^{\ell+m+1}). \tag{60}$$

Methods for the extrapolation of power series will be treated later.

3.4. Aitken process

The special case $\varepsilon_2^{(n)} = e_1(s_n)$ is identical to the famous Δ^2 method of Aitken [2]

$$s_n^{(1)} = s_n - \frac{(s_{n+1} - s_n)^2}{s_{n+2} - 2s_{n+1} + s_n} \tag{61}$$

with kernel

$$s_n = s + c(s_{n+1} - s_n), \quad n \in \mathbb{N}_0. \tag{62}$$

Iteration of the Δ^2 method yields the iterated Aitken process [14,84,102]

$$\begin{aligned} \mathbf{A}_n^{(0)} &= s_n, \\ \mathbf{A}_n^{(k+1)} &= \mathbf{A}_n^{(k)} - \frac{(\mathbf{A}_{n+1}^{(k)} - \mathbf{A}_n^{(k)})^2}{\mathbf{A}_{n+2}^{(k)} - 2\mathbf{A}_{n+1}^{(k)} + \mathbf{A}_n^{(k)}}. \end{aligned} \tag{63}$$

The iterated Aitken process and the epsilon algorithm accelerate linear convergence and can sometimes be applied successfully for the summation of alternating divergent series.

3.5. Overholt process

The Overholt process is defined by the recursive scheme [64]

$$\begin{aligned} V_n^{(0)}(\{\{s_n\}\}) &= s_n, \\ V_n^{(k)}(\{\{s_n\}\}) &= \frac{(\Delta s_{n+k-1})^k V_{n+1}^{(k-1)}(\{\{s_n\}\}) - (\Delta s_{n+k})^k V_n^{(k-1)}(\{\{s_n\}\})}{(\Delta s_{n+k-1})^k - (\Delta s_{n+k})^k} \end{aligned} \tag{64}$$

for $k \in \mathbb{N}$ and $n \in \mathbb{N}_0$. It is important for the convergence acceleration of fixed point iterations.

4. Levin-type sequence transformations

4.1. Definitions for Levin-type transformations

A set $\Lambda^{(k)} = \{\lambda_{n,j}^{(k)} \in \mathbb{K} \mid n \in \mathbb{N}_0, 0 \leq j \leq k\}$ is called a *coefficient set of order k* with $k \in \mathbb{N}$ if $\lambda_{n,k}^{(k)} \neq 0$ for all $n \in \mathbb{N}_0$. Also, $\Lambda = \{\Lambda^{(k)} \mid k \in \mathbb{N}\}$ is called *coefficient set*. Two coefficient sets

$A = \{\{\lambda_{n,j}^{(k)}\}\}$ and $\hat{A} = \{\{\hat{\lambda}_{n,j}^{(k)}\}\}$ are called *equivalent*, if for all n and k , there is a constant $c_n^{(k)} \neq 0$ such that $\hat{\lambda}_{n,j}^{(k)} = c_n^{(k)} \lambda_{n,j}^{(k)}$ for all j with $0 \leq j \leq k$.

For each coefficient set $A^{(k)} = \{\lambda_{n,j}^{(k)} | n \in \mathbb{N}_0, 0 \leq j \leq k\}$ of order k , one may define a *Levin-type sequence transformation of order k* by

$$\begin{aligned} \mathcal{T}[A^{(k)}] : \mathbb{S}^{\mathbb{K}} \times \mathbb{Y}^{(k)} &\rightarrow \mathbb{S}^{\mathbb{K}} \\ &: (\{\{s_n\}\}, \{\{\omega_n\}\}) \mapsto \{\{s'_n\}\} = \mathcal{T}[A^{(k)}](\{\{s_n\}\}, \{\{\omega_n\}\}) \end{aligned} \tag{65}$$

with

$$s'_n = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{\sum_{j=0}^k \lambda_{n,j}^{(k)} s_{n+j} / \omega_{n+j}}{\sum_{j=0}^k \lambda_{n,j}^{(k)} / \omega_{n+j}} \tag{66}$$

and

$$\mathbb{Y}^{(k)} = \left\{ \{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}} : \sum_{j=0}^k \lambda_{n,j}^{(k)} / \omega_{n+j} \neq 0 \text{ for all } n \in \mathbb{N}_0 \right\}. \tag{67}$$

We call $\mathcal{T}[A] = \{\mathcal{T}[A^{(k)}] | k \in \mathbb{N}\}$ the Levin-type sequence transformation corresponding to the coefficient set $A = \{A^{(k)} | k \in \mathbb{N}\}$. We write $\mathcal{T}^{(k)}$ and \mathcal{T} instead of $\mathcal{T}[A^{(k)}]$ and $\mathcal{T}[A]$, respectively, whenever the coefficients $\lambda_{n,j}^{(k)}$ are clear from the context. Also, if two coefficient sets A and \hat{A} are equivalent, they give rise to the same sequence transformation, i.e., $\mathcal{T}[A] = \mathcal{T}[\hat{A}]$, since

$$\frac{\sum_{j=0}^k \hat{\lambda}_{n,j}^{(k)} s_{n+j} / \omega_{n+j}}{\sum_{j=0}^k \hat{\lambda}_{n,j}^{(k)} / \omega_{n+j}} = \frac{\sum_{j=0}^k \lambda_{n,j}^{(k)} s_{n+j} / \omega_{n+j}}{\sum_{j=0}^k \lambda_{n,j}^{(k)} / \omega_{n+j}} \quad \text{for } \hat{\lambda}_{n,j}^{(k)} = c_n^{(k)} \lambda_{n,j}^{(k)} \tag{68}$$

with arbitrary $c_n^{(k)} \neq 0$.

The number $\mathcal{T}_n^{(k)}$ are often arranged in a two-dimensional table

$$\begin{array}{cccc} \mathcal{T}_0^{(0)} & \mathcal{T}_0^{(1)} & \mathcal{T}_0^{(2)} & \dots \\ \mathcal{T}_1^{(0)} & \mathcal{T}_1^{(1)} & \mathcal{T}_1^{(2)} & \dots \\ \mathcal{T}_2^{(0)} & \mathcal{T}_2^{(1)} & \mathcal{T}_2^{(2)} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{array} \tag{69}$$

that is called the \mathcal{T} table. The transformations $\mathcal{T}^{(k)}$ thus correspond to columns, i.e., to following vertical paths in the table. The numerators and denominators such that $\mathcal{T}_n^{(k)} = N_n^{(k)} / D_n^{(k)}$ also are often arranged in analogous N and D tables.

Note that for fixed N , one may also define a transformation

$$\mathcal{T}_N : \{\{s_{n+N}\}\} \mapsto \{\{\mathcal{T}_N^{(k)}\}\}_{k=0}^{\infty}. \tag{70}$$

This corresponds to horizontal paths in the \mathcal{T} table. These are sometimes called diagonals, because rearranging the table in such a way that elements with constant values of $n + k$ are members of the same row, $\mathcal{T}_N^{(k)}$ for fixed N correspond to diagonals of the rearranged table.

For a given coefficient set A define the *moduli* by

$$\mu_n^{(k)} = \max_{0 \leq j \leq k} \{|\lambda_{n,j}^{(k)}|\} \tag{71}$$

and the characteristic polynomials by

$$\Pi_n^{(k)} \in \mathbb{P}^{(k)}: \Pi_n^{(k)}(z) = \sum_{j=0}^k \lambda_{n,j}^{(k)} z^j \tag{72}$$

for $n \in \mathbb{N}_0$ and $k \in \mathbb{N}$.

Then, $\mathcal{T}[A]$ is said to be *in normalized form* if $\mu_n^{(k)} = 1$ for all $k \in \mathbb{N}$ and $n \in \mathbb{N}_0$. Is is said to be *in subnormalized form* if for all $k \in \mathbb{N}$ there is a constant $\tilde{\mu}^{(k)}$ such that $\mu_n^{(k)} \leq \tilde{\mu}^{(k)}$ for all $n \in \mathbb{N}_0$.

Any Levin-type sequence transformation $\mathcal{T}[A]$ can rewritten in normalized form. To see this, use

$$c_n^{(k)} = 1/\mu_n^{(k)} \tag{73}$$

in Eq. (68). Similarly, each Levin-type sequence transformation can be rewritten in (many different) subnormalized forms.

A Levin-type sequence transformation of order k is said to be *convex* if $\Pi_n^{(k)}(1) = 0$ for all $n \in \mathbb{N}_0$. Equivalently, it is convex if $\{\{1\}\} \notin \mathbb{Y}^{(k)}$, i.e., if the transformation vanishes for $\{\{s_n\}\} = \{\{c\omega_n\}\}$, $c \in \mathbb{K}$. Also, $\mathcal{T}[A]$ is called convex, if $\mathcal{T}[A^{(k)}]$ is convex for all $k \in \mathbb{N}$. We will see that this property is important for ensuring convergence acceleration for linearly convergent sequences.

A given Levin-type transformation \mathcal{T} can also be rewritten as

$$\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \sum_{j=0}^k \gamma_{n,j}^{(k)}(\omega_n) s_{n+j}, \quad \omega_n = (\omega_n, \dots, \omega_{n+k}) \tag{74}$$

with

$$\gamma_{n,j}^{(k)}(\omega_n) = \frac{\lambda_{n,j}^{(k)}}{\omega_{n+j}} \left[\sum_{j'=0}^k \frac{\lambda_{n,j'}^{(k)}}{\omega_{n+j'}} \right]^{-1}, \quad \sum_{j=0}^k \gamma_{n,j}^{(k)}(\omega_n) = 1. \tag{75}$$

Then, one may define *stability indices* by

$$\Gamma_n^{(k)}(\mathcal{T}) = \sum_{j=0}^k |\gamma_{n,j}^{(k)}(\omega_n)| \geq 1. \tag{76}$$

Note that any sequence transformation \mathcal{Q}

$$\mathcal{Q}_n^{(k)} = \sum_{j=0}^k q_{n,j}^{(k)} s_{n+j} \tag{77}$$

with

$$\sum_{j=0}^k q_{n,j}^{(k)} = 1 \tag{78}$$

can formally be rewritten as a Levin-type sequence transformation according to $\mathcal{Q}_n^{(k)} = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\})$ with coefficients $\lambda_{n,j}^{(k)} = \omega_{n+j} q_{n,j}^{(k)} \rho_n^{(k)}$ where the validity of Eq. (78) requires to set

$$\rho_n^{(k)} = \sum_{j=0}^k \lambda_{n,j}^{(k)} / \omega_{n+j}. \tag{79}$$

If for given $k \in \mathbb{N}$ and for a transformation $\mathcal{T}[A^{(k)}]$ the following limits exist and have the values:

$$\lim_{n \rightarrow \infty} \lambda_{n,j}^{(k)} = \overset{\circ}{\lambda}_j^{(k)} \quad (80)$$

for all $0 \leq j \leq k$, and if $\overset{\circ}{A}^{(k)}$ is a coefficient set of order k which means that at least the limit $\overset{\circ}{\lambda}_k^{(k)}$ does not vanish, then a limiting transformation $\overset{\circ}{\mathcal{T}}[\overset{\circ}{A}^{(k)}]$ exists where $\overset{\circ}{A}^{(k)} = \{\overset{\circ}{\lambda}_j^{(k)}\}$. More explicitly, we have

$$\begin{aligned} \overset{\circ}{\mathcal{T}}[A^{(k)}]: \mathbb{S}^{\mathbb{K}} \times \overset{\circ}{\mathbb{Y}}^{(k)} &\rightarrow \mathbb{S}^{\mathbb{K}} \\ &: (\{\{s_n\}\}, \{\{\omega_n\}\}) \mapsto \{\{s'_n\}\} \end{aligned} \quad (81)$$

with

$$s'_n = \overset{\circ}{\mathcal{T}}^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} s_{n+j} / \omega_{n+j}}{\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} / \omega_{n+j}} \quad (82)$$

and

$$\overset{\circ}{\mathbb{Y}}^{(k)} = \left\{ \{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}} : \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} / \omega_{n+j} \neq 0 \text{ for all } n \in \mathbb{N}_0 \right\}. \quad (83)$$

Obviously, this limiting transformation itself is a Levin-type sequence transformation and automatically is given in subnormalized form.

4.1.1. Variants of Levin-type transformations

For the following, assume that $\beta > 0$ is an arbitrary constant, $a_n = \Delta s_{n-1}$, and \hat{a}_n are Kummer-related to the a_n with limit or antilimit \hat{s} (cf. Section 2.2.1).

A variant of a Levin-type sequence transformation \mathcal{T} is obtained by a particular choice ω_n . For $\omega_n = f_n(\{\{s_n\}\})$, the transformation \mathcal{T} is nonlinear in the s_n . In particular, we have [50,53,79]:

t Variant:

$${}^t\omega_n = \Delta s_{n-1} = a_n: {}^t\mathcal{T}_n^{(k)}(\{\{s_n\}\}) = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{{}^t\omega_n\}\}). \quad (84)$$

u Variant:

$${}^u\omega_n = (n + \beta) \Delta s_{n-1} = (n + \beta)a_n: {}^u\mathcal{T}_n^{(k)}(\beta, \{\{s_n\}\}) = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{{}^u\omega_n\}\}). \quad (85)$$

v Variant:

$${}^v\omega_n = -\frac{\Delta s_{n-1} \Delta s_n}{\Delta^2 s_{n-1}} = \frac{a_n a_{n+1}}{a_n - a_{n+1}}: {}^v\mathcal{T}_n^{(k)}(\{\{s_n\}\}) = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{{}^v\omega_n\}\}). \quad (86)$$

tilde Variant:

$$\tilde{\omega}_n = \Delta s_n = a_{n+1}: \tilde{\mathcal{T}}_n^{(k)}(\{\{s_n\}\}) = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\tilde{\omega}_n\}\}). \quad (87)$$

lt Variant:

$${}^{lt}\omega_n = \hat{a}_n: {}^{lt}\mathcal{T}_n^{(k)}(\{\{s_n\}\}) = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{{}^{lt}\omega_n\}\}). \quad (88)$$

lu Variant:

$${}^{lu}\omega_n = (n + \beta)\hat{a}_n: {}^{lu}\mathcal{F}_n^{(k)}(\beta, \{\{s_n\}\}) = \mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{{}^{lu}\omega_n\}\}). \tag{89}$$

lv Variant:

$${}^{lv}\omega_n = \frac{\hat{a}_n\hat{a}_{n+1}}{\hat{a}_n - \hat{a}_{n+1}}: {}^{lv}\mathcal{F}_n^{(k)}(\{\{s_n\}\}) = \mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{{}^{lv}\omega_n\}\}). \tag{90}$$

li Variant:

$${}^{li}\omega_n = \hat{a}_{n+1}: {}^{li}\mathcal{F}_n^{(k)}(\{\{s_n\}\}) = \mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{{}^{li}\omega_n\}\}). \tag{91}$$

K Variant:

$${}^K\omega_n = \hat{s}_n - \hat{s}: {}^K\mathcal{F}_n^{(k)}(\{\{s_n\}\}) = \mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{{}^K\omega_n\}\}). \tag{92}$$

The *K* variant of a Levin-type transformation \mathcal{F} is linear in the s_n . This holds also for the *lt*, *lu*, *lv* and *li* variants.

4.2. Important examples of Levin-type sequence transformations

In this section, we present important Levin-type sequence transformations. For each transformation, we give the definition, recursive algorithms and some background information.

4.2.1. \mathcal{J} transformation

The \mathcal{J} transformation was derived and studied by Homeier [35,36,38–40,46]. Although the \mathcal{J} transformation was derived by hierarchically consistent iteration of the simple transformation

$$s'_n = s_{n+1} - \omega_{n+1} \frac{\Delta s_n}{\Delta \omega_n}, \tag{93}$$

it was possible to derive an explicit formula for its kernel as is discussed later. It may be defined via the recursive scheme

$$\begin{aligned} N_n^{(0)} &= s_n/\omega_n, & D_n^{(0)} &= 1/\omega_n, \\ N_n^{(k)} &= \nabla_n^{(k-1)}N_n^{(k-1)}, & D_n^{(k)} &= \nabla_n^{(k-1)}D_n^{(k-1)}, \\ \mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{\delta_n^{(k)}\}\}) &= N_n^{(k)}/D_n^{(k)}, \end{aligned} \tag{94}$$

where the generalized difference operator defined in Eq. (33) involves quantities $\delta_n^{(k)} \neq 0$ for $k \in \mathbb{N}_0$. Special cases of the \mathcal{J} transformation result from corresponding choices of the $\delta_n^{(k)}$. These are summarized in Table 1.

Using generalized difference operators $\nabla_n^{(k)}$, we also have the representation [36, Eq. (38)]

$$\mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{\delta_n^{(k)}\}\}) = \frac{\nabla_n^{(k-1)}\nabla_n^{(k-2)}\dots\nabla_n^{(0)}[s_n/\omega_n]}{\nabla_n^{(k-1)}\nabla_n^{(k-2)}\dots\nabla_n^{(0)}[1/\omega_n]}. \tag{95}$$

The \mathcal{J} transformation may also be computed using the alternative recursive schemes [36,46]

$$\begin{aligned} \hat{D}_n^{(0)} &= 1/\omega_n, & \hat{N}_n^{(0)} &= s_n/\omega_n, \\ \hat{D}_n^{(k)} &= \Phi_n^{(k-1)}\hat{D}_{n+1}^{(k-1)} - \hat{D}_n^{(k-1)}, & k &\in \mathbb{N}, \\ \hat{N}_n^{(k)} &= \Phi_n^{(k-1)}\hat{N}_{n+1}^{(k-1)} - \hat{N}_n^{(k-1)}, & k &\in \mathbb{N}, \end{aligned} \tag{96}$$

Table 1
Special cases of the \mathcal{J} transformation^a

Case	$\psi_j(n)^b$	$\delta_n^{(k)c}$
Drummond transformation $\mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\})$	n^j	1
Homeier \mathcal{J} transformation $\mathcal{J}_n^{(k)}(\alpha, \{\{s_n\}\}, \{\{\omega_n\}\}, \{\Delta_n^{(k)}\})$ $= \mathcal{J}_n^{(2k)}(\{\{s_n\}\}, \{\{e^{-i\alpha n} \omega_n\}\}, \{\delta_n^{(k)}\})$	Eq. (231)	$\delta_n^{(2\ell)} = \exp(2i\alpha n),$ $\delta_n^{(2\ell+1)} = \exp(-2i\alpha n)\Delta_n^{(\ell)}$
Homeier \mathcal{F} transformation $\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{x_n\}\})$	$1/(x_n)_j$	$\frac{x_{n+k+1}-x_n}{x_{n+k}-1} \prod_{j=0}^{n-1} \frac{(x_j+k)(x_{j+k+1}+k-1)}{(x_j+k-1)(x_{j+k+2}+k)}$
Homeier ${}_p\mathbf{J}$ transformation ${}_p\mathbf{J}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\})$	Eq. (231)	$\frac{1}{(n+\beta+(p-1)k)_2}$
Levin transformation $\mathcal{L}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\})$	$(n+\beta)^{-j}$	$\frac{1}{(n+\beta)(n+\beta+k+1)}$
generalized \mathcal{L} transformation $\mathcal{L}_n^{(k)}(\alpha, \beta, \{\{s_n\}\}, \{\{\omega_n\}\})$	$(n+\beta)^{-j\alpha}$	$\frac{(n+\beta+k+1)^2 - (n+\beta)^2}{(n+\beta)^2(n+\beta+k+1)^2}$
Levin-Sidi $d^{(1)}$ transformation [22,54,77] $(d^{(1)})_n^{(k)}(\alpha, \{\{s_n\}\})$	$(R_n + \alpha)^{-j}$	$\frac{1}{R_{n+k+1} + \alpha} - \frac{1}{R_n + \alpha}$
Mosig–Michalski algorithm [60,61] $M_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{x_n\}\})$	Eq. (231)	$\frac{1}{x_n^2} \left(1 - \frac{\omega_n x_{n+1}^{2k}}{\omega_{n+1} x_n^{2k}} \right)$
Sidi W algorithm (GREP ⁽¹⁾) [73,77,78] $W_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{t_n\}\})$	t_n^j	$t_{n+k+1} - t_n$
Weniger \mathcal{C} transformation [87] $\mathcal{C}_n^{(k)}(\gamma, \beta/\gamma, \{\{s_n\}\}, \{\{\omega_n\}\})$	$\frac{1}{(\gamma n + \beta)_j}$	$\frac{(n+1+(\beta+k-1)/\gamma)_k}{(n+(\beta+k)/\gamma)_{k+2}}$
Weniger \mathcal{M} transformation $\mathcal{M}_n^{(k)}(\xi, \{\{s_n\}\}, \{\{\omega_n\}\})$	$\frac{1}{(-n-\xi)_j}$	$\frac{(n+1+\xi-(k-1))_k}{(n+\xi-k)_{k+2}}$
Weniger \mathcal{S} transformation $\mathcal{S}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\})$	$1/(n+\beta)_j$	$\frac{1}{(n+\beta+2k)_2}$
Iterated Aitken process [2,84] $\mathbf{A}_n^{(k)}(\{\{s_n\}\})$ $= \mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\Delta s_n\}\}, \{\delta_n^{(k)}\})$	Eq. (231)	$\frac{(\Delta \mathbf{A}_n^{(k+1)}(\{\{s_n\}\}))(\Delta^2 \mathbf{A}_n^{(k)}(\{\{s_n\}\}))}{(\Delta \mathbf{A}_n^{(k)}(\{\{s_n\}\}))(\Delta \mathbf{A}_{n+1}^{(k)}(\{\{s_n\}\}))}$
Overholt process [64] $V_n^{(k)}(\{\{s_n\}\})$ $= \mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\Delta s_n\}\}, \{\delta_n^{(k)}\})$	Eq. (231)	$\frac{(\Delta s_{n+k+1})\Delta[(\Delta s_{n+k})^{k+1}]}{(\Delta s_{n+k})^{k+1}}$

^aRefs. [36,38,40].

^bFor the definition of the $\psi_{j,n}$ see Eq. (5).

^cFactors independent of n are irrelevant.

$$\mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\delta_n^{(k)}\}) = \frac{\hat{N}_n^{(k)}}{\hat{D}_n^{(k)}}$$

with

$$\Phi_n^{(0)} = 1, \quad \Phi_n^{(k)} = \frac{\delta_n^{(0)} \delta_n^{(1)} \dots \delta_n^{(k-1)}}{\delta_{n+1}^{(0)} \delta_{n+1}^{(1)} \dots \delta_{n+1}^{(k-1)}}, \quad k \in \mathbb{N} \tag{97}$$

and

$$\begin{aligned} \tilde{D}_n^{(0)} &= 1/\omega_n, \quad \tilde{N}_n^{(0)} = s_n/\omega_n, \\ \tilde{D}_n^{(k)} &= \tilde{D}_{n+1}^{(k-1)} - \Psi_n^{(k-1)} \tilde{D}_n^{(k-1)}, \quad k \in \mathbb{N}, \\ \tilde{N}_n^{(k)} &= \tilde{N}_{n+1}^{(k-1)} - \Psi_n^{(k-1)} \tilde{N}_n^{(k-1)}, \quad k \in \mathbb{N}, \end{aligned} \tag{98}$$

$$\mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\delta_n^{(k)}\}) = \frac{\tilde{N}_n^{(k)}}{\tilde{D}_n^{(k)}}$$

with

$$\Psi_n^{(0)} = 1, \quad \Psi_n^{(k)} = \frac{\delta_{n+k}^{(0)} \delta_{n+k-1}^{(1)} \dots \delta_{n+1}^{(k-1)}}{\delta_{n+k-1}^{(0)} \delta_{n+k-2}^{(1)} \dots \delta_n^{(k-1)}}, \quad k \in \mathbb{N}. \tag{99}$$

The quantities $\Psi_n^{(k)}$ should not be mixed up with the $\Psi_{k,n}(u)$ as defined in Eq. (43).

As shown in [46], the coefficients for the algorithm (96) that are defined via $\hat{D}_n^{(k)} = \sum_{j=0}^k \lambda_{n,j}^{(k)}/\omega_{n+j}$, satisfy the recursion

$$\lambda_{n,j}^{(k+1)} = \Phi_n^{(k)} \lambda_{n+1,j-1}^{(k)} - \lambda_{n,j}^{(k)} \tag{100}$$

with starting values $\lambda_{n,j}^{(0)} = 1$. This holds for all j if we define $\lambda_{n,j}^{(k)} = 0$ for $j < 0$ or $j > k$. Because $\Phi_n^{(k)} \neq 0$, we have $\lambda_{n,k}^{(k)} \neq 0$ such that $\{\lambda_{n,j}^{(k)}\}$ is a coefficient set for all $k \in \mathbb{N}_0$.

Similarly, the coefficients for algorithm (98) that are defined via $\tilde{D}_n^{(k)} = \sum_{j=0}^k \tilde{\lambda}_{n,j}^{(k)}/\omega_{n+j}$, satisfy the recursion

$$\tilde{\lambda}_{n,j}^{(k+1)} = \tilde{\lambda}_{n+1,j-1}^{(k)} - \Psi_n^{(k)} \tilde{\lambda}_{n,j}^{(k)} \tag{101}$$

with starting values $\tilde{\lambda}_{n,j}^{(0)} = 1$. This holds for all j if we define $\tilde{\lambda}_{n,j}^{(k)} = 0$ for $j < 0$ or $j > k$. In this case, we have $\tilde{\lambda}_{n,k}^{(k)} = 1$ such that $\{\tilde{\lambda}_{n,j}^{(k)}\}$ is a coefficient set for all $k \in \mathbb{N}_0$.

Since the \mathcal{J} transformation vanishes for $\{\{s_n\}\} = \{\{c\omega_n\}\}$, $c \in \mathbb{K}$ according to Eq. (95) for all $k \in \mathbb{N}$, it is convex. This may also be shown by using induction in k using $\lambda_{n,1}^{(1)} = -\lambda_{n,0}^{(1)} = 1$ and the equation

$$\sum_{j=0}^{k+1} \lambda_{n,j}^{(k+1)} = \Phi_n^{(k)} \sum_{j=0}^k \lambda_{n+1,j}^{(k)} - \sum_{j=0}^k \lambda_{n,j}^{(k)} \tag{102}$$

that follows from Eq. (100).

Assuming that the limits $\Phi_k = \lim_{n \rightarrow \infty} \Phi_n^{(k)}$ exist for all $k \in \mathbb{N}$ and noting that for $k = 0$ always $\Phi_0 = 1$ holds, it follows that there exists a limiting transformation $\overset{\circ}{\mathcal{J}}[\overset{\circ}{A}]$ that can be considered as special variant of the \mathcal{J} transformation and with coefficients given explicitly as [46, Eq. (16)]

$$\overset{\circ}{\lambda}_j^{(k)} = (-1)^{k-j} \sum_{\substack{j_0+j_1+\dots+j_{k-1}=j \\ j_0 \in \{0,1\}, \dots, j_{k-1} \in \{0,1\}}} \prod_{m=0}^{k-1} (\Phi_m)^{j_m}. \tag{103}$$

As characteristic polynomial we obtain

$$\overset{\circ}{\Pi}^{(k)}(z) = \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} z^j = \prod_{j=0}^{k-1} (\Phi_j z - 1). \tag{104}$$

Hence, the $\overset{\circ}{\mathcal{J}}$ transformation is convex since $\overset{\circ}{\Pi}^{(k)}(1) = 0$ due to $\Phi_0 = 1$.

The ${}_p\mathbf{J}$ Transformation: This is the special case of the \mathcal{J} transformation corresponding to

$$\delta_n^{(k)} = \frac{1}{(n + \beta + (p - 1)k)_2} \tag{105}$$

or to [46, Eq. (18)]²

$$\Phi_n^{(k)} = \begin{cases} \left(\frac{n + \beta + 2}{p - 1}\right)_k / \left(\frac{n + \beta}{p - 1}\right)_k & \text{for } p \neq 1, \\ \left(\frac{n + \beta + 2}{n + \beta}\right)^k & \text{for } p = 1 \end{cases} \tag{106}$$

or to

$$\Psi_n^{(k)} = \begin{cases} \left(\frac{n + \beta + k - 1}{p - 2}\right)_k / \left(\frac{n + \beta + k + 1}{p - 2}\right)_k & \text{for } p \neq 2, \\ \left(\frac{n + \beta + k - 1}{n + \beta + k + 1}\right)^k & \text{for } p = 2, \end{cases} \tag{107}$$

that is,

$${}_p\mathbf{J}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{1/(n + \beta + (p - 1)k)_2\}). \tag{108}$$

The limiting transformation ${}_p\overset{\circ}{\mathbf{J}}$ of the ${}_p\mathbf{J}$ transformation exists for all p and corresponds to the $\overset{\circ}{\mathcal{J}}$ transformation with $\Phi_k = 1$ for all k in \mathbb{N}_0 . This is exactly the Drummond transformation discussed in Section 4.2.2, i.e., we have

$${}_p\overset{\circ}{\mathbf{J}}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}). \tag{109}$$

² The equation in [46] contains an error.

4.2.2. Drummond transformation

This transformation was given by Drummond [19]. It was also discussed by Weniger [84]. It may be defined as

$$\mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{\Delta^k [s_n/\omega_n]}{\Delta^k [1/\omega_n]}. \tag{110}$$

Using the definition (32) of the forward difference operator, the coefficients may be taken as

$$\lambda_{n,j}^{(k)} = (-1)^j \binom{k}{j}, \tag{111}$$

i.e., independent of n . As moduli, one has $\mu_n^{(k)} = \binom{k}{[k/2]} = \tilde{\mu}^{(k)}$. Consequently, the Drummond transformation is given in subnormalized form. As characteristic polynomial we obtain

$$\Pi_n^{(k)}(z) = \sum_{j=0}^k (-1)^j \binom{k}{j} z^j = (1 - z)^k. \tag{112}$$

Hence, the Drummond transformation is convex since $\Pi_n^{(k)}(1) = 0$. Interestingly, the Drummond transformation is identical to its limiting transformation:

$$\overset{\circ}{\mathcal{D}}^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}). \tag{113}$$

The Drummond transformation may be computed using the recursive scheme

$$\begin{aligned} N_n^{(0)} &= s_n/\omega_n, & D_n^{(0)} &= 1/\omega_n, \\ N_n^{(k)} &= \Delta N_n^{(k-1)}, & D_n^{(k)} &= \Delta D_n^{(k-1)}, \\ \mathcal{D}_n^{(k)} &= N_n^{(k)}/D_n^{(k)}. \end{aligned} \tag{114}$$

4.2.3. Levin transformation

This transformation was given by Levin [53]. It was also discussed by Weniger [84]. It may be defined as³

$$\mathcal{L}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{(n + \beta + k)^{1-k} \Delta^k [(n + \beta)^{k-1} s_n/\omega_n]}{(n + \beta + k)^{1-k} \Delta^k [(n + \beta)^{k-1}/\omega_n]}. \tag{115}$$

Using the definition (32) of the forward difference operator, the coefficients may be taken as

$$\lambda_{n,j}^{(k)} = (-1)^j \binom{k}{j} (n + \beta + j)^{k-1} / (n + \beta + k)^{k-1}. \tag{116}$$

The moduli satisfy $\mu_n^{(k)} \leq \binom{k}{[k/2]} = \tilde{\mu}^{(k)}$ for given k . Consequently, the Levin transformation is given in subnormalized form. As characteristic polynomial we obtain

$$\Pi_n^{(k)}(z) = \sum_{j=0}^k (-1)^j \binom{k}{j} z^j (n + \beta + j)^{k-1} / (n + \beta + k)^{k-1}. \tag{117}$$

³ Note that the order of indices is different from that in the literature.

Since $\Pi_n^{(k)}(1) = 0$ because Δ^k annihilates any polynomial in n with degree less than k , the Levin transformation is convex. The limiting transformation is identical to the Drummond transformation

$$\mathcal{L}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}). \tag{118}$$

The Levin transformation may be computed using the recursive scheme [21,55,84,14, Section 2.7]

$$\begin{aligned} N_n^{(0)} &= s_n/\omega_n, & D_n^{(0)} &= 1/\omega_n, \\ N_n^{(k)} &= N_{n+1}^{(k-1)} - \frac{(\beta+n)(\beta+n+k-1)^{k-2}}{(\beta+n+k)^{k-1}} N_n^{(k-1)}, \\ D_n^{(k)} &= D_{n+1}^{(k-1)} - \frac{(\beta+n)(\beta+n+k-1)^{k-2}}{(\beta+n+k)^{k-1}} D_n^{(k-1)}, \\ \mathcal{L}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\}) &= N_n^{(k)}/D_n^{(k)}. \end{aligned} \tag{119}$$

This is essentially the same as the recursive scheme (98) for the \mathcal{J} transformation with

$$\Psi_n^{(k)} = \frac{(\beta+n)(\beta+n+k)^{k-1}}{(\beta+n+k+1)^k}, \tag{120}$$

since the Levin transformation is a special case of the \mathcal{J} transformation (see Table 1). Thus, the Levin transformation can also be computed recursively using scheme (94)

$$\delta_n^{(k)} = \frac{1}{(n+\beta)(n+\beta+k+1)} \tag{121}$$

or scheme (96) with [46]

$$\Phi_n^{(k)} = (n+\beta+k+1) \frac{(n+\beta+1)^{k-1}}{(n+\beta)^k}. \tag{122}$$

4.2.4. Weniger transformations

Weniger [84,87,88] derived sequence transformations related to factorial series. These may be regarded as special cases of the transformation

$$\mathcal{C}_n^{(k)}(\alpha, \zeta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{((\alpha[n+\zeta+k])_{k-1})^{-1} \Delta^k [(\alpha[n+\zeta])_{k-1} s_n/\omega_n]}{((\alpha[n+\zeta+k])_{k-1})^{-1} \Delta^k [(\alpha[n+\zeta])_{k-1}/\omega_n]}. \tag{123}$$

In particular, the Weniger \mathcal{S} transformation may be defined as

$$\mathcal{S}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{C}_n^{(k)}(1, \beta, \{\{s_n\}\}, \{\{\omega_n\}\}) \tag{124}$$

and the Weniger \mathcal{M} transformation as

$$\mathcal{M}_n^{(k)}(\zeta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{C}_n^{(k)}(-1, \zeta, \{\{s_n\}\}, \{\{\omega_n\}\}). \tag{125}$$

The parameters β , ζ , and ζ are taken to be positive real numbers. Weniger considered the \mathcal{C} transformation only for $\alpha > 0$ [87,88] and thus, he was not considering the \mathcal{M} transformation as a special case of the \mathcal{C} transformation. He also found that one should choose $\zeta \geq k - 1$. In the u variant of the \mathcal{M} transformation he proposed to choose $\omega_n = (-n - \zeta) \Delta s_{n-1}$. This variant is denoted as ${}^u\mathcal{M}$ transformation in the present work.

Using the definition (32) of the forward difference operator, the coefficients may be taken as

$$\lambda_{n,j}^{(k)} = (-1)^j \binom{k}{j} (\alpha[n + \zeta + j])_{k-1} / (\alpha[n + \zeta + k])_{k-1} \quad (126)$$

in the case of the \mathcal{C} transformation, as

$$\lambda_{n,j}^{(k)} = (-1)^j \binom{k}{j} (n + \beta + j)_{k-1} / (n + \beta + k)_{k-1} \quad (127)$$

in the case of the \mathcal{S} transformation, and as

$$\lambda_{n,j}^{(k)} = (-1)^j \binom{k}{j} (-n - \xi - j)_{k-1} / (-n - \xi - k)_{k-1} \quad (128)$$

in the case of the \mathcal{M} transformation.

The \mathcal{S} transformation in (124) may be computed using the recursive scheme (98) with [84, Section 8.3]

$$\Psi_n^{(k)} = \frac{(\beta + n + k)(\beta + n + k - 1)}{(\beta + n + 2k)(\beta + n + 2k - 1)}. \quad (129)$$

The \mathcal{M} transformation in (125) may be computed using the recursive scheme (98) with [84, Section 9.3]

$$\Psi_n^{(k)} = \frac{\xi + n - k + 1}{\xi + n + k + 1}. \quad (130)$$

The \mathcal{C} transformation in (123) may be computed using the recursive scheme (98) with [87, Eq. (3.3)]

$$\Psi_n^{(k)} = (\alpha[\zeta + n] + k - 2) \frac{(\alpha[n + \zeta + k - 1])_{k-2}}{(\alpha[n + \zeta + k])_{k-1}}. \quad (131)$$

Since the operator Δ^k for $k \in \mathbb{N}$ annihilates all polynomials in n of degree smaller than k , the transformations \mathcal{S} , \mathcal{M} , and \mathcal{C} are convex. The moduli satisfy $\mu_n^{(k)} \leq \binom{k}{\lfloor k/2 \rfloor} = \tilde{\mu}^{(k)}$ for given k . Consequently, the three Weniger transformations are given in subnormalized form.

For $\alpha \rightarrow \infty$, the Levin transformation is obtained from the \mathcal{C} transformation [87]. The \mathcal{S} transformation is identical to the ${}_3\mathbf{J}$ transformation. It is also the special case $x_n = n + \beta$ of the \mathcal{F} transformation. Analogously, the \mathcal{C} transformation is obtained for $x_n = \alpha[\zeta + n]$. All these Weniger transformations are special cases of the \mathcal{J} transformation (cf Table 1).

The limiting transformation of all these Weniger transformations is the Drummond transformation.

4.2.5. Levin–Sidi transformations and W algorithms

As noted above in Section 3.2, the $d^{(m)}$ transformations were introduced by Levin and Sidi [54] as a generalization of the u variant of the Levin transformation, and these transformations may be implemented recursively using the $\mathbf{W}^{(m)}$ algorithms.

The case $m = 1$ corresponding to the $d^{(1)}$ transformation and the $\mathbf{W}^{(1)} = W$ algorithm is relevant for the present survey of Levin-type transformations. In the following, the k th-order transformation $\mathcal{T}^{(k)}$ of Levin-type transformation \mathcal{T} as given by the W algorithm is denoted by $W^{(k)}$ which should not be confused with the $\mathbf{W}^{(m)}$ algorithms of Ford and Sidi [22].

The W algorithm [73] was also studied by other authors [84, Section 7.4], [14, p. 71f, 116f] and may be regarded as a special case of the \mathcal{J} transformation [36]. It may be defined as (cf [78, Theorems 1.1 and 1.2])

$$\begin{aligned}
 N_n^{(0)} &= \frac{s_n}{\omega_n}, & D_n^{(0)} &= \frac{1}{\omega_n}, \\
 N_n^{(k)} &= \frac{N_{n+1}^{(k-1)} - N_n^{(k-1)}}{t_{n+k} - t_n}, \\
 D_n^{(k)} &= \frac{D_{n+1}^{(k-1)} - D_n^{(k-1)}}{t_{n+k} - t_n}, \\
 W_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{t_n\}\}) &= N_n^{(k)} / D_n^{(k)}
 \end{aligned} \tag{132}$$

and computes

$$W_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{t_n\}\}) = \frac{\square_n^{(k)}(s_n/\omega_n)}{\square_n^{(k)}(1/\omega_n)}, \tag{133}$$

where the divided difference operators $\square_n^{(k)} = \square_n^{(k)}[\{\{t_n\}\}]$ are used. The W algorithm may be used to calculate the Levin transformation on putting $t_n = 1/(n + \beta)$. Some authors call a linear variant of the W algorithm with $\omega_n = (-1)^{n+1} e^{-n\zeta} t_n^\alpha$ the W transformation, while the \tilde{t} variant of the W algorithm [74,75] is sometimes called mW transformation [31,57,60].

If $t_{n+1}/t_n \rightarrow \tau$ for large n , one obtains as limiting transformation the $\overset{\circ}{\mathcal{J}}$ transformation with $\Phi_j = \tau^{-j}$ and characteristic polynomial

$$\overset{\circ}{\Pi}^{(k)}(z) = \prod_{j=0}^{k-1} (z/\tau^j - 1). \tag{134}$$

For the $d^{(1)}$ transformation, we write

$$(d^{(1)})_n^{(k)}(\alpha, \{\{s_n\}\}, \{\{\xi_n\}\}) = W_n^{(k)}(\{\{s_{\xi_n}\}\}, \{\{(\xi_n + \alpha)(s_{\xi_n} - s_{\xi_{n-1}})\}\}, \{\{1/(\xi_n + \alpha)\}\}). \tag{135}$$

Thus, it corresponds to the variant of the W algorithm with remainder estimates chosen as $(\xi_n + \alpha)(s_{\xi_n} - s_{\xi_{n-1}})$ operating on the subsequence $\{\{s_{\xi_n}\}\}$ of $\{\{s_n\}\}$ with $t_n = 1/(\xi_n + \alpha)$. It should be noted that this is not(!) identical to the u variant

$${}^u W_n^{(k)}(\{\{s_{\xi_n}\}\}, \{\{1/(\xi_n + \alpha)\}\}) = W_n^{(k)}(\{\{s_{\xi_n}\}\}, \{\{{}^u\omega_n\}\}, \{\{1/(\xi_n + \alpha)\}\}), \tag{136}$$

neither for ${}^u\omega_n = (n + \alpha)(s_{\xi_n} - s_{\xi_{n-1}})$ nor for ${}^u\omega_n = (\xi_n + \alpha)(s_{\xi_n} - s_{\xi_{n-1}})$, since the remainder estimates are chosen differently in Eq. (135).

The $d^{(1)}$ transformation was thoroughly analyzed by Sidi (see [77,78] and references therein).

4.2.6. Mosig–Michalski transformation

The Mosig–Michalski transformation — also known as “weighted–averages algorithm” — was introduced by Mosig [61] and modified later by Michalski who gave the \tilde{t} variant of the transformation the name \mathcal{H} transformation (that is used for a different transformation in the present article(!)), and applied it to the computation of Sommerfeld integrals [60].

The Mosig–Michalski transformation M may be defined via the recursive scheme

$$\begin{aligned}
 s_n^{(0)} &= s_n, \\
 s_n^{(k+1)} &= \frac{s_n^{(k)} + \eta_n^{(k)} s_{n+1}^{(k)}}{1 + \eta_n^{(k)}}, \\
 M_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{x_n\}\}) &= s_n^{(k)}
 \end{aligned}
 \tag{137}$$

for $n \in \mathbb{N}_0$ and $k \in \mathbb{N}_0$ where $\{\{x_n\}\}$ is an auxiliary sequence with $\lim_{n \rightarrow \infty} 1/x_n = 0$ such that $x_{n+\ell} > x_n$ for $\ell \in \mathbb{N}_0$ and $x_0 > 1$, i.e., a diverging sequence of monotonously increasing positive numbers, and

$$\eta_n^{(k)} = -\frac{\omega_n}{\omega_{n+1}} \left(\frac{x_{n+1}}{x_n} \right)^{2k}.
 \tag{138}$$

Putting $\omega_n^{(k)} = \omega_n/x_n^{2k}$, $N_n^{(k)} = s_n^{(k)}/\omega_n^{(k)}$, and $D_n^{(k)} = 1/\omega_n^{(k)}$, it is easily seen that the recursive scheme (137) is equivalent to the scheme (94) with

$$\delta_n^{(k)} = \frac{1}{x_n^2} \left(1 - \frac{\omega_n x_{n+1}^{2k}}{\omega_{n+1} x_n^{2k}} \right).
 \tag{139}$$

Thus, the Mosig–Michalski transformation is a special case of the \mathcal{J} transformation. Its character as a Levin-type transformation is somewhat formal since the $\delta_n^{(k)}$ and, hence, the coefficients $\lambda_{n,j}^{(k)}$ depend on the ω_n .

If $x_{n+1}/x_n \sim \zeta > 1$ for large n , then a limiting transformation exists, namely $M(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{\zeta^{n+1}\}\})$. It corresponds to the \mathcal{J} transformation with $\Phi_k = \zeta^{2k}$. This may be seen by putting $\hat{D}_n^{(k)} = 1/\omega_n$, $\hat{N}_n^{(k)} = s_n^{(k)} D_n^{(k)}$ and $\hat{\Phi}_n^{(k)} = \zeta^{2k}$ in Eq. (96).

4.2.7. \mathcal{F} transformation

This transformation is seemingly new. It will be derived in a later section. It may be defined as

$$\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{x_n\}\}) = \frac{\square_n^{(k)}((x_n)_{k-1} s_n / \omega_n)}{\square_n^{(k)}((x_n)_{k-1} / \omega_n)} = \frac{x_n^k / (x_n)_{k-1} \square_n^{(k)}((x_n)_{k-1} s_n / \omega_n)}{x_n^k / (x_n)_{k-1} \square_n^{(k)}((x_n)_{k-1} / \omega_n)},
 \tag{140}$$

where $\{\{x_n\}\}$ is an auxiliary sequence with $\lim_{n \rightarrow \infty} 1/x_n = 0$ such that $x_{n+\ell} > x_n$ for $\ell \in \mathbb{N}$ and $x_0 > 1$, i.e., a diverging sequence of monotonously increasing positive numbers. Using the definition (39) of the divided difference operator $\square_n^{(k)} = \square_n^{(k)}[\{\{x_n\}\}]$, the coefficients may be taken as

$$\lambda_{n,j}^{(k)} = \frac{(x_{n+j})_{k-1}}{(x_n)_{k-1}} \prod_{\substack{i=0 \\ i \neq j}}^k \frac{x_n}{x_{n+j} - x_{n+i}} = \prod_{\substack{m=0 \\ m \neq j}}^{k-2} \frac{x_{n+j} + m}{x_n + m} \left(\frac{x_n}{x_{n+j}} \right)^k \prod_{\substack{i=0 \\ i \neq j}}^k \frac{1}{1 - x_{n+i}/x_{n+j}}.
 \tag{141}$$

Assuming that the following limit exists such that

$$\lim_{n \rightarrow \infty} \frac{x_{n+1}}{x_n} = \zeta > 1
 \tag{142}$$

holds, we see that one can define a limiting transformation $\overset{\circ}{\mathcal{F}}^{(k)}$ with coefficients

$$\overset{\circ}{\lambda}_j^{(k)} = \lim_{n \rightarrow \infty} \lambda_{n,j}^{(k)} = \frac{1}{\zeta^j} \prod_{\substack{\ell=0 \\ \ell \neq j}}^k \frac{1}{1 - \zeta^{\ell-j}} = (-1)^k \zeta^{-k(k+1)/2} \prod_{\substack{\ell=0 \\ \ell \neq j}}^k \frac{1}{\zeta^{-j} - \zeta^{-\ell}}, \tag{143}$$

since

$$\prod_{m=0}^{k-2} \frac{x_{n+j} + m}{x_n + m} \left(\frac{x_n}{x_{n+j}} \right)^k \prod_{\substack{\ell=0 \\ \ell \neq j}}^k \frac{1}{1 - x_{n+\ell}/x_{n+j}} \rightarrow \zeta^{(k-1)j} \zeta^{k(-j)} \prod_{\substack{\ell=0 \\ \ell \neq j}}^k \frac{\zeta^{-\ell}}{\zeta^{-\ell} - \zeta^{-j}} \tag{144}$$

for $n \rightarrow \infty$. Thus, the limiting transformation is given by

$$\overset{\circ}{\mathcal{F}}^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \zeta) = \frac{\sum_{j=0}^k s_{n+j}/\omega_{n+j} \prod_{\substack{\ell=0 \\ \ell \neq j}}^k 1/(\zeta^{-j} - \zeta^{-\ell})}{\sum_{j=0}^k \frac{1}{\omega_{n+j}} \prod_{\substack{\ell=0 \\ \ell \neq j}}^k 1/(\zeta^{-j} - \zeta^{-\ell})}. \tag{145}$$

Comparison with definition (39) of the divided difference operators reveals that the limiting transformation can be rewritten as

$$\overset{\circ}{\mathcal{F}}^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \zeta) = \frac{\square_n^{(k)}[\{\{\zeta^{-n}\}\}](s_n/\omega_n)}{\square_n^{(k)}[\{\{\zeta^{-n}\}\}](1/\omega_n)}. \tag{146}$$

Comparison to Eq. (133) shows that the limiting transformation is nothing but the W algorithm for $t_n = \zeta^{-n}$. As characteristic polynomial we obtain

$$\overset{\circ}{\Pi}^{(k)}(z) = \sum_{j=0}^k z^j \prod_{\substack{\ell=0 \\ \ell \neq j}}^k \frac{1}{\zeta^{-j} - \zeta^{-\ell}} = \zeta^{k(k+1)/2} \prod_{j=0}^{k-1} \frac{1 - z\zeta^j}{\zeta^{j+1} - 1}. \tag{147}$$

The last equality is easily proved by induction. Hence, the $\overset{\circ}{\mathcal{F}}$ transformation is convex since $\overset{\circ}{\Pi}^{(k)}(1) = 0$.

As shown in Appendix B, the \mathcal{F} transformation may be computed using the recursive scheme

$$\begin{aligned} N_n^{(0)} &= \frac{1}{x_n - 1} \frac{s_n}{\omega_n}, & D_n^{(0)} &= \frac{1}{x_n - 1} \frac{1}{\omega_n}, \\ N_n^{(k)} &= \frac{(x_{n+k} + k - 2)N_{n+1}^{(k-1)} - (x_n + k - 2)N_n^{(k-1)}}{x_{n+k} - x_n}, \\ D_n^{(k)} &= \frac{(x_{n+k} + k - 2)D_{n+1}^{(k-1)} - (x_n + k - 2)D_n^{(k-1)}}{x_{n+k} - x_n}, \\ \overset{\circ}{\mathcal{F}}_n^{(k)} &= N_n^{(k)}/D_n^{(k)}. \end{aligned} \tag{148}$$

It follows directly from Eq. (146) and the recursion relation for divided differences that the limiting transformation can be computed via the recursive scheme

$$\begin{aligned} \overset{\circ}{N}_n^{(0)} &= \frac{s_n}{\omega_n}, & \overset{\circ}{D}_n^{(0)} &= \frac{1}{\omega_n}, \\ \overset{\circ}{N}_n^{(k)} &= \frac{\overset{\circ}{N}_{n+1}^{(k-1)} - \overset{\circ}{N}_n^{(k-1)}}{\zeta^{-(n+k)} - \zeta^{-n}}, \end{aligned}$$

$$\begin{aligned} \overset{\circ}{D}_n^{(k)} &= \frac{\overset{\circ}{D}_{n+1}^{(k-1)} - \overset{\circ}{D}_n^{(k-1)}}{\zeta^{-(n+k)} - \zeta^{-n}}, \\ \overset{\circ}{\mathcal{F}}_n^{(k)} &= \overset{\circ}{N}_n^{(k)} / \overset{\circ}{D}_n^{(k)}. \end{aligned} \tag{149}$$

4.2.8. $\mathcal{J}\mathcal{D}$ transformation

This transformation is newly introduced in this article. In Section 5.2.1, it is derived via (asymptotically) hierarchically consistent iteration of the $\mathcal{D}^{(2)}$ transformation, i.e., of

$$s'_n = \frac{\Delta^2(s_n/\omega_n)}{\Delta^2(1/\omega_n)}. \tag{150}$$

The $\mathcal{J}\mathcal{D}$ transformation may be defined via the recursive scheme

$$\begin{aligned} N_n^{(0)} &= s_n/\omega_n, \quad D_n^{(0)} = 1/\omega_n, \\ N_n^{(k)} &= \tilde{\nabla}_n^{(k-1)} N_n^{(k-1)}, \quad D_n^{(k)} = \tilde{\nabla}_n^{(k-1)} D_n^{(k-1)}, \\ \mathcal{J}\mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\zeta_n^{(k)}\}) &= N_n^{(k)} / D_n^{(k)}, \end{aligned} \tag{151}$$

where the generalized difference operator defined in Eq. (34) involves quantities $\zeta_n^{(k)} \neq 0$ for $k \in \mathbb{N}_0$. Special cases of the $\mathcal{J}\mathcal{D}$ transformation result from corresponding choices of the $\zeta_n^{(k)}$. From Eq. (151) one easily obtains the alternative representation

$$\mathcal{J}\mathcal{D}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\zeta_n^{(k)}\}) = \frac{\tilde{\nabla}_n^{(k-1)} \tilde{\nabla}_n^{(k-2)} \dots \tilde{\nabla}_n^{(0)} [s_n/\omega_n]}{\tilde{\nabla}_n^{(k-1)} \tilde{\nabla}_n^{(k-2)} \dots \tilde{\nabla}_n^{(0)} [1/\omega_n]}. \tag{152}$$

Thus, the $\mathcal{J}\mathcal{D}^{(k)}$ is a Levin-type sequence transformation of order $2k$.

4.2.9. \mathcal{H} transformation and generalized \mathcal{H} transformation

The \mathcal{H} transformation was introduced by Homeier [34] and used or studied in a series of articles [35,41–44,63]. Target of the \mathcal{H} transformation are Fourier series

$$s = A_0/2 + \sum_{j=1}^{\infty} (A_j \cos(j\alpha) + B_j \sin(j\alpha)) \tag{153}$$

with partial sums $s_n = A_0/2 + \sum_{j=1}^n (A_j \cos(j\alpha) + B_j \sin(j\alpha))$ where the Fourier coefficients A_n and B_n have asymptotic expansions of the form

$$C_n \sim \rho^n n^\varepsilon \sum_{j=0}^{\infty} c_j n^{-j} \tag{154}$$

for $n \rightarrow \infty$ with $\rho \in \mathbb{K}$, $\varepsilon \in \mathbb{K}$ and $c_0 \neq 0$.

The \mathcal{H} transformation was criticized by Sidi [77] as very unstable and useless near singularities of the Fourier series. However, Sidi failed to notice that – as in the case of the $d^{(1)}$ transformation with $\xi_n = \tau n$ – one can apply also the \mathcal{H} transformation (and also most other Levin-type sequence transformations) to the subsequence $\{\{s_{\xi_n}\}\}$ of $\{\{s_n\}\}$. The new sequence elements $s_{\xi_n} = s_{\tau n}$ can be regarded as the partial sums of a Fourier series with τ -fold frequency. Using this τ -fold frequency approach, one can obtain stable and accurate convergence acceleration even in the vicinity of singularities [41–44].

The \mathcal{H} transformation may be defined as

$$\begin{aligned}
 N_n^{(0)} &= (n + \beta)^{-1} s_n / \omega_n, & D_n^{(0)} &= (n + \beta)^{-1} / \omega_n, \\
 N_n^{(k)} &= (n + \beta)N_n^{(k-1)} + (n + 2k + \beta)N_{n+2}^{(k-1)} - 2 \cos(\alpha)(n + k + \beta)N_{n+1}^{(k-1)}, \\
 D_n^{(k)} &= (n + \beta)D_n^{(k-1)} + (n + 2k + \beta)D_{n+2}^{(k-1)} - 2 \cos(\alpha)(n + k + \beta)D_{n+1}^{(k-1)}, \\
 \mathcal{H}_n^{(k)}(\alpha, \beta, \{\{s_n\}\}, \{\{\omega_n\}\}) &= N_n^{(k)} / D_n^{(k)},
 \end{aligned} \tag{155}$$

where $\cos \alpha \neq \pm 1$ and $\beta \in \mathbb{R}_+$.

It can also be represented in the explicit form [34]

$$\mathcal{H}_n^{(k)}(\alpha, \beta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{\mathcal{P}[P^{(2k)}(\alpha)][(n + \beta)^{k-1} s_n / \omega_n]}{\mathcal{P}[P^{(2k)}(\alpha)][(n + \beta)^{k-1} / \omega_n]}, \tag{156}$$

where the $P_m^{(2k)}(\alpha)$ and the polynomial $P^{(2k)}(\alpha) \in \mathcal{P}^{(2k)}$ are defined via

$$P^{(2k)}(\alpha)(x) = (x^2 - 2x \cos \alpha + 1)^k = \sum_{m=0}^{2k} P_m^{(2k)}(\alpha)x^m \tag{157}$$

and \mathcal{P} is the polynomial operator defined in Eq. (38). This shows that the $\mathcal{H}^{(k)}$ transformation is a Levin-type transformation of order $2k$. It is not convex.

A subnormalized form is

$$\mathcal{H}_n^{(k)}(\alpha, \beta, \{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{\sum_{m=0}^{2k} P_m^{(2k)}(\alpha) \frac{(n+\beta+m)^{k-1}}{(n+\beta+2k)^{k-1}} \frac{s_{n+m}}{\omega_{n+m}}}{\sum_{m=0}^{2k} P_m^{(2k)}(\alpha) \frac{(n+\beta+m)^{k-1}}{(n+\beta+2k)^{k-1}} \frac{1}{\omega_{n+m}}}. \tag{158}$$

This relation shows that the limiting transformation

$$\mathcal{H}^{(k)} = \frac{\mathcal{P}[P^{(2k)}(\alpha)][s_n / \omega_n]}{\mathcal{P}[P^{(2k)}(\alpha)][1 / \omega_n]} \tag{159}$$

exists, and has characteristic polynomial $P^{(2k)}(\alpha)$.

A generalized \mathcal{H} transformation was defined by Homeier [40,43]. It is given in terms of the polynomial $P^{(k,M)}(\mathbf{e}) \in \mathbb{P}^{(kM)}$ with

$$P^{(k,M)}(\mathbf{e})(x) = \prod_{m=1}^M (x - e_m)^k = \sum_{\ell=0}^{kM} p_\ell^{(k,M)}(\mathbf{e})x^\ell, \tag{160}$$

where $\mathbf{e} = (e_1, \dots, e_M) \in \mathbb{K}^M$ is a vector of constant parameters. Then, the generalized \mathcal{H} transformation is defined as

$$\mathcal{H}_n^{(k,M)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\}, \mathbf{e}) = \frac{\mathcal{P}[P^{(k,M)}(\mathbf{e})][(n + \beta)^{k-1} s_n / \omega_n]}{\mathcal{P}[P^{(k,M)}(\mathbf{e})][(n + \beta)^{k-1} / \omega_n]}. \tag{161}$$

This shows that the generalized $\mathcal{H}^{(k,M)}$ is a Levin-type sequence transformation of order kM . The generalized \mathcal{H} transformation can be computed recursively using the scheme [40,43]

$$\begin{aligned} N_n^{(0)} &= (n + \beta)^{-1} s_n / \omega_n, & D_n^{(0)} &= (n + \beta)^{-1} / \omega_n, \\ N_n^{(k)} &= \sum_{j=0}^M q_j (n + \beta + jk) N_{n+j}^{(k-1)}, \\ D_n^{(k)} &= \sum_{j=0}^M q_j (n + \beta + jk) D_{n+j}^{(k-1)}, \end{aligned} \tag{162}$$

$$\mathcal{H}_n(k, M)(\beta, \{s_n\}, \{\omega_n\}, \mathbf{e}) = \frac{N_n^{(k)}}{D_n^{(k)}}.$$

Here, the q_j are defined by

$$\prod_{m=1}^M (x - e_m) = \sum_{j=0}^M q_j x^j. \tag{163}$$

Algorithm (155) is a special case of algorithm (162). To see this, one observes that $M = 2$, $e_1 = \exp(i\alpha)$ und $e_2 = \exp(-i\alpha)$ imply $q_0 = q_2 = 1$ and $q_1 = -2 \cos(\alpha)$.

For $M = 1$ and $e_1 = 1$, the Levin transformation is recovered.

4.2.10. \mathcal{I} transformation

The \mathcal{I} transformation was in a slightly different form introduced by Homeier [35]. It was derived via (asymptotically) hierarchically consistent iteration of the $\mathcal{H}^{(1)}$ transformation, i.e., of

$$s'_n = \frac{s_{n+2}/\omega_{n+2} - 2 \cos(\alpha) s_{n+1}/\omega_{n+1} + s_n/\omega_n}{1/\omega_{n+2} - 2 \cos(\alpha)/\omega_{n+1} + 1/\omega_n}. \tag{164}$$

For the derivation and an analysis of the properties of the \mathcal{I} transformation see [40,44]. The \mathcal{I} transformation may be defined via the recursive scheme

$$\begin{aligned} N_n^{(0)} &= s_n / \omega_n, & D_n^{(0)} &= 1 / \omega_n, \\ N_n^{(k+1)} &= \nabla_n^{(k)}[\alpha] N_n^{(k)}, \\ D_n^{(k+1)} &= \nabla_n^{(k)}[\alpha] D_n^{(k)}, \end{aligned} \tag{165}$$

$$\mathcal{I}_n^{(k)}(\alpha, \{s_n\}, \{\omega_n\}, \{\Delta_n^{(k)}\}) = \frac{N_n^{(k)}}{D_n^{(k)}},$$

where the generalized difference operator $\nabla_n^{(k)}[\alpha]$ defined in Eq. (35) involves quantities $\Delta_n^{(k)} \neq 0$ for $k \in \mathbb{N}_0$. Special cases of the \mathcal{I} transformation result from corresponding choices of the $\Delta_n^{(k)}$. From Eq. (165) one easily obtains the alternative representation

$$\mathcal{I}_n^{(k)}(\{s_n\}, \{\omega_n\}, \{\Delta_n^{(k)}\}) = \frac{\nabla_n^{(k-1)}[\alpha] \nabla_n^{(k-2)}[\alpha] \dots \nabla_n^{(0)}[\alpha] [s_n/\omega_n]}{\nabla_n^{(k-1)}[\alpha] \nabla_n^{(k-2)}[\alpha] \dots \nabla_n^{(0)}[\alpha] [1/\omega_n]}. \tag{166}$$

Thus, $\mathcal{I}^{(k)}$ is a Levin-type sequence transformation of order $2k$. It is not convex.

Put $\Theta_n^{(0)} = 1$ and for $k > 0$ define

$$\Theta_n^{(k)} = \frac{\Delta_n^{(0)} \dots \Delta_n^{(k-1)}}{\Delta_{n+1}^{(0)} \dots \Delta_{n+1}^{(k-1)}}. \tag{167}$$

If for all $k \in \mathbb{N}$ the limits

$$\lim_{n \rightarrow \infty} \Theta_n^{(k)} = \Theta_k \tag{168}$$

exist (we have always $\Theta_0 = 1$), then one can define a limiting transformation $\overset{\circ}{\mathcal{J}}$ for large n . It is a special case of the \mathcal{J} transformation according to [44]

$$\overset{\circ}{\mathcal{J}}_n^{(k)}(\alpha, \{\{s_n\}\}, \{\{\omega_n\}\}, \{\{\Theta_k\}\}) = \mathcal{J}_n^{(k)}(\alpha, \{\{s_n\}\}, \{\{\omega_n\}\}, \{\{(\Theta_k/\Theta_{k+1})^n\}\}). \tag{169}$$

This is a transformation of order $2k$. The characteristic polynomials of $\overset{\circ}{\mathcal{J}}$ are known [44] to be

$$\mathcal{Q}^{(2k)}(\alpha) \in \mathbb{P}^{2k}: \mathcal{Q}^{(2k)}(\alpha)(z) = \prod_{j=0}^{k-1} [(1 - z\Theta_j \exp(i\alpha))(1 - z\Theta_j \exp(-i\alpha))]. \tag{170}$$

4.2.11. \mathcal{K} transformation

The \mathcal{K} transformation was introduced by Homeier [37] in a slightly different form. It was obtained via iteration of the simple transformation

$$s'_n = \frac{\zeta_n^{(0)}s_n/\omega_n + \zeta_n^{(1)}s_{n+1}/\omega_{n+1} + \zeta_n^{(2)}s_{n+2}/\omega_{n+2}}{\zeta_n^{(0)}1/\omega_n + \zeta_n^{(1)}1/\omega_{n+1} + \zeta_n^{(2)}1/\omega_{n+2}}, \tag{171}$$

that is exact for sequences of the form

$$s_n = s + \omega_n(cP_n + dQ_n), \tag{172}$$

where c and d are arbitrary constants, while P_n and Q_n are two linearly independent solutions of the three-term recurrence

$$\zeta_n^{(0)}v_n + \zeta_n^{(1)}v_{n+1} + \zeta_n^{(2)}v_{n+2} = 0. \tag{173}$$

The \mathcal{K} transformation may be defined via the recursive scheme

$$\begin{aligned} N_n^{(0)} &= s_n/\omega_n, & D_n^{(0)} &= 1/\omega_n, \\ N_n^{(k+1)} &= \partial_n^{(k)}[\zeta]N_n^{(k)}, \\ D_n^{(k+1)} &= \partial_n^{(k)}[\zeta]D_n^{(k)}, \end{aligned} \tag{174}$$

$$\mathcal{K}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\tilde{\Delta}_n^{(k)}\}, \{\{\zeta_n^{(j)}\}\}) = \frac{N_n^{(k)}}{D_n^{(k)}},$$

where the generalized difference operator $\partial_n^{(k)}[\zeta]$ defined in Eq. (36) involves recursion coefficients $\zeta_{n+k}^{(j)}$ with $j = 0, 1, 2$ and quantities $\tilde{\Delta}_n^{(k)} \neq 0$ for $k \in \mathbb{N}_0$. Special cases of the \mathcal{K} transformation for given recursion, i.e., for given $\zeta_n^{(j)}$, result from corresponding choices of the $\tilde{\Delta}_n^{(k)}$. From Eq. (174) one easily obtains the alternative representation

$$\mathcal{K}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\tilde{\Delta}_n^{(k)}\}, \{\{\zeta_n^{(j)}\}\}) = \frac{\partial_n^{(k-1)}[\zeta]\partial_n^{(k-2)}[\zeta] \dots \partial_n^{(0)}[\zeta][s_n/\omega_n]}{\partial_n^{(k-1)}[\zeta]\partial_n^{(k-2)}[\zeta] \dots \partial_n^{(0)}[\zeta][1/\omega_n]}. \tag{175}$$

Thus, $\mathcal{H}^{(k)}$ is a Levin-type sequence transformation of order $2k$. It is not convex. For applications of the \mathcal{H} transformation see [37,40,42,45].

5. Methods for the construction of Levin-type transformations

In this section, we discuss approaches for the construction of Levin-type sequence transformations and point out the relation to their kernel.

5.1. Model sequences and annihilation operators

As discussed in the introduction, the derivation of sequence transformations may be based on model sequences. These may be of the form (10) or of the form (6). Here, we consider model sequences of the latter type that involves remainder estimates ω_n . As described in Section 3.1, determinantal representations for the corresponding sequence transformations can be derived using Cramer’s rule, and one of the recursive schemes of the **E** algorithm may be used for the computation. However, for important special choices of the functions $\psi_j(n)$, simpler recursive schemes and more explicit representations in the form (11) can be obtained using the annihilation operator approach of Weniger [84]. This approach was also studied by Brezinski and Matos [13] who showed that it leads to a unified derivation of many extrapolation algorithms and related devices and general results about their kernels. Further, we mention the work of Matos [59] who analysed the approach further and derived a number of convergence acceleration results for Levin-type sequence transformations.

In this approach, an annihilation operator $\mathcal{A} = \mathcal{A}_n^{(k)}$ as defined in Eq. (31) is needed that annihilates the sequences $\{\{\psi_j(n)\}\}$, i.e., such that

$$\mathcal{A}_n^{(k)}(\{\{\psi_j(n)\}\}) = 0 \quad \text{for } j = 0, \dots, k - 1. \tag{176}$$

Rewriting Eq. (6) in the form

$$\frac{\sigma_n - \sigma}{\omega_n} = \sum_{j=0}^{k-1} c_j \psi_j(n) \tag{177}$$

and applying \mathcal{A} to both sides of this equation, one sees that

$$\mathcal{A}_n^{(k)} \left\{ \left\{ \frac{\sigma_n - \sigma}{\omega_n} \right\} \right\} = 0 \tag{178}$$

This equation may be solved for σ due to the linearity of \mathcal{A} . The result is

$$\sigma = \frac{\mathcal{A}_n^{(k)}(\{\{\sigma_n/\omega_n\}\})}{\mathcal{A}_n^{(k)}(\{\{1/\omega_n\}\})} \tag{179}$$

leading to a sequence transformation

$$\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega\}\}) = \frac{\mathcal{A}_n^{(k)}(\{\{s_n/\omega_n\}\})}{\mathcal{A}_n^{(k)}(\{\{1/\omega_n\}\})}. \tag{180}$$

Since \mathcal{A} is linear, this transformation can be rewritten in the form (11), i.e., a Levin-type transformation has been obtained.

We note that this process can be reversed, that is, for each Levin-type sequence transformation $\mathcal{T}[A^{(k)}]$ of order k there is an annihilation operator, namely the polynomial operator $\mathcal{P}[\Pi_n^{(k)}]$ as defined in Eq. (38) where $\Pi_n^{(k)}$ are the characteristic polynomials as defined in Eq. (72). Using this operator, the defining Eq. (66) can be rewritten as

$$\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \frac{\mathcal{P}[\Pi_n^{(k)}](s_n/\omega_n)}{\mathcal{P}[\Pi_n^{(k)}](1/\omega_n)}. \tag{181}$$

Let $\phi_{n,m}(k)$ for $m = 0, \dots, k - 1$ be k linearly independent solutions of the linear $(k + 1)$ -term recurrence

$$\sum_{j=0}^k \lambda_{n,j}^{(k)} v_{n+j} = 0. \tag{182}$$

Then $\mathcal{P}[\Pi_n^{(k)}]\phi_{n,m}(k) = 0$ for $m = 0, \dots, k - 1$, i.e., $\mathcal{P}[\Pi_n^{(k)}]$ is an annihilation operator for all solutions of Eq. (182). Thus, all sequences that are annihilated by this operator are linear combinations of the k sequences $\{\{\phi_{n,m}^{(k)}\}\}$.

If $\{\{\sigma_n\}\}$ is a sequence in the kernel of $\mathcal{T}^{(k)}$ with (anti)limit σ , we must have

$$\sigma = \frac{\mathcal{P}[\Pi_n^{(k)}](\sigma_n/\omega_n)}{\mathcal{P}[\Pi_n^{(k)}](1/\omega_n)} \tag{183}$$

or after some rearrangement using the linearity of \mathcal{P}

$$\mathcal{P}[\Pi_n^{(k)}] \left(\frac{\sigma_n - \sigma}{\omega_n} \right) = 0. \tag{184}$$

Hence, we must have

$$\frac{\sigma_n - \sigma}{\omega_n} = \sum_{m=0}^{k-1} c_m \phi_{n,m}^{(k)}, \tag{185}$$

or, equivalently

$$\sigma_n = \sigma + \omega_n \sum_{m=0}^{k-1} c_m \phi_{n,m}^{(k)} \tag{186}$$

for some constants c_m . Thus, we have determined the kernel of $\mathcal{T}^{(k)}$ that can also be considered as the set of model sequences for this transformation. Thus, we have proved the following theorem:

Theorem 1. *Let $\phi_{n,m}^{(k)}$ for $m = 0, \dots, k - 1$ be the k linearly independent solutions of the linear $(k + 1)$ -term recurrence (182). The kernel of $\mathcal{T}[A^{(k)}](\{\{s_n\}\}, \{\{\omega_n\}\})$ is given by all sequences $\{\{\sigma_n\}\}$ with (anti)limit σ and elements σ_n of the form (186) for arbitrary constants c_m .*

We note that the $\psi_j(n)$ for $j = 0, \dots, k - 1$ can essentially be identified with the $\phi_{n,j}^{(k)}$. Thus, we have determinantal representations for known $\psi_j(n)$ as noted above in the context of the E algorithm. See also [38] for determinantal representations of the \mathcal{J} transformations and the relation to its kernel.

Examples of annihilation operators and the functions $\psi_j(n)$ that are annihilated are given in Table 2. Examples for the Levin-type sequence transformations that have been derived using the approach of model sequences are discussed in Section 5.1.2.

Table 2
Examples of annihilation operators^a

Type	Operator	$\psi_j(n), j = 0, \dots, k - 1$
Differences	Δ^k	$(n + \beta)^j$ $(n + \beta)_j$ $(\alpha[n + \zeta])^j$ $(\alpha[n + \zeta])_j$
Weighted differences	$\Delta^k(n + \beta)^{k-1}$ $\Delta^k(n + \beta)_{k-1}$ $\Delta^k(\alpha[n + \zeta])^{k-1}$ $\Delta^k(\alpha[n + \zeta])_{k-1}$	$p_j(n), p_j \in \mathbb{P}^{(j)}$ $1/(n + \beta)^j$ $1/(n + \beta)_j$ $1/(\alpha[n + \zeta])^j$ $1/(\alpha[n + \zeta])_j$
Divided differences	$\square_n^{(k)}[\{\{t_n\}\}]$ $\square_n^{(k)}[\{\{t_n\}\}]$ $\square_n^{(k)}[\{\{x_n\}\}](x_n)_{k-1}$	t_n^j $p_j(t_n), p_j \in \mathbb{P}^{(j)}$ $1/(x_n)_j$
Polynomial	$\mathcal{P}[P^{(2k)}(\alpha)]$ $\mathcal{P}[P^{(2k)}(\alpha)](n + \beta)^{k-1}$ $\mathcal{P}[P^{(2k)}(\alpha)](n + \beta)_{k-1}$ $\mathcal{P}[P^{(k)}]$ $\mathcal{P}[P^{(k)}](n + \beta)^m$ L_1 (see (188)) L_2 (see (189)) \tilde{L} (see (191))	$\exp(+ian)p_j(n), p_j \in \mathbb{P}^{(j)}$ $\exp(-ian)p_j(n), p_j \in \mathbb{P}^{(j)}$ $\exp(+ian)/(n + \beta)^j$ $\exp(-ian)/(n + \beta)^j$ $\exp(+ian)/(n + \beta)_j$ $\exp(-ian)/(n + \beta)_j$ $\psi_j(n)$ is solution of $\sum_{m=0}^k P_n^{(k)} v_{n+j} = 0$ $(n + \beta)^m \psi_j(n)$ is solution of $\sum_{m=0}^k P_n^{(k)} v_{n+j} = 0$ $\frac{\alpha^{n+1}}{n!}$ $\frac{n! \alpha^{n+1}}{n^j \alpha^{n+1}}$ $\frac{\Gamma(n+2j+1)}{n!}$

^aSee also Section 5.1.1.

Note that the annihilation operators used by Weniger [84,87,88] were weighted difference operators $\mathcal{W}_n^{(k)}$ as defined in Eq. (37). Homeier [36,38,39] discussed operator representations for the \mathcal{J} transformation that are equivalent to many of the annihilation operators and related sequence transformations as given by Brezinski and Matos [13]. The latter have been further discussed by Matos [59] who considered among others Levin-type sequence transformations with constant coefficients, $\lambda_{n,j}^{(k)} = \text{const.}$, and with polynomial coefficients $\lambda_{n,j}^{(k)} = \lambda_j(n + 1)$, with $\lambda_j \in \mathbb{P}$, and $n \in \mathbb{N}_0$, in particular annihilation operators of the form

$$L(u_n) = (\Omega^l + \lambda_1 \Omega^{l-1} + \dots + \lambda_l)(u_n) \tag{187}$$

with the special cases

$$L_1(u_n) = (\Omega - \alpha_1)(\Omega - \alpha_2) \dots (\Omega - \alpha_l)(u_n) \quad (\alpha_i \neq \alpha_j \text{ for all } i \neq j) \tag{188}$$

and

$$L_2(u_n) = (\Omega - \alpha)^l(u_n), \tag{189}$$

where

$$\Omega^r(u_n) = (n + 1)_r u_{n+r}, \quad n \in \mathbb{N}_0 \tag{190}$$

and

$$\tilde{L}(u_n) = (\pi - \alpha_1)(\pi - \alpha_2) \cdots (\pi - \alpha_l)(u_n), \tag{191}$$

where

$$\pi(u_n) = (n + 1) \Delta u_n, \quad \pi^r(u_n) = \pi(\pi^{r-1}(u_n)), \quad n \in \mathbb{N}_0 \tag{192}$$

and the λ 's and α 's are constants. Note that n is shifted in comparison to [59] where the convention $n \in \mathbb{N}$ was used. See also Table 2 for the corresponding annihilated functions $\psi_f(n)$.

Matos [59] also considered difference operators of the form

$$L(u_n) = \Delta^k + p_{k-1}(n) \Delta^{k-1} + \cdots + p_1(n) \Delta + p_0(n), \tag{193}$$

where the functions f_j given by $f_j(t) = p_j(1/t)t^{-k+j}$ for $j = 0, \dots, k - 1$ are analytic in the neighborhood of 0. For such operators, there is no explicit formula for the functions that are annihilated. However, the asymptotic behavior of such functions is known [6,59]. We will later return to such annihilation operators and state some convergence results.

5.1.1. Derivation of the \mathcal{F} transformation

As an example for the application of the annihilation operator approach, we derive the \mathcal{F} transformation. Consider the model sequence

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j \frac{1}{(x_n)_j}, \tag{194}$$

that may be rewritten as

$$\frac{\sigma_n - \sigma}{\omega_n} = \sum_{j=0}^{k-1} c_j \frac{1}{(x_n)_j}. \tag{195}$$

We note that Eq. (194) corresponds to modeling $\mu_n = R_n/\omega_n$ as a truncated factorial series in x_n (instead as a truncated power series as in the case of the W algorithm). The x_n are elements of $\{\{x_n\}\}$ an auxiliary sequence $\{\{x_n\}\}$ such that $\lim_{n \rightarrow \infty} 1/x_n = 0$ and also $x_{n+\ell} > x_n$ for $\ell \in \mathbb{N}$ and $x_0 > 1$, i.e., a diverging sequence of monotonously increasing positive numbers. To find an annihilation operator for the $\psi_f(n) = 1/(x_n)_j$, we make use of the fact that the divided difference operator $\square_n^{(k)} = \square_n^{(k)}[\{\{x_n\}\}]$ annihilates polynomials in x_n of degree less than k . Also, we observe that the definition of the Pochhammer symbols entails that

$$(x_n)_{k-1}/(x_n)_j = (x_n + j)_{k-1-j} \tag{196}$$

is a polynomial of degree less than k in x_n for $0 \leq j \leq k - 1$. Thus, the sought annihilation operator is $\mathcal{A} = \square_n^{(k)}(x_n)_{k-1}$ because

$$\square_n^{(k)}(x_n)_{k-1} \frac{1}{(x_n)_j} = 0, \quad 0 \leq j < k. \tag{197}$$

Hence, for the model sequence (194), one can calculate σ via

$$\sigma = \frac{\square_n^{(k)}((x_n)_{k-1}\sigma_n/\omega_n)}{\square_n^{(k)}((x_n)_{k-1}/\omega_n)} \quad (198)$$

and the \mathcal{F} transformation (140) results by replacing σ_n by s_n in the right-hand side of Eq. (198).

5.1.2. Important special cases

Here, we collect model sequences and annihilation operators for some important Levin-type sequence transformations that were derived using the model sequence approach. For further examples see also [13]. The model sequences are the kernels by construction. In Section 5.2.2, kernels and annihilation operators are stated for important Levin-type transformation that were derived using iterative methods.

Levin transformation: The model sequence for $\mathcal{L}^{(k)}$ is

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j / (n + \beta)^j. \quad (199)$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \Delta^k (n + \beta)^{k-1}. \quad (200)$$

Weniger transformations: The model sequence for $\mathcal{S}^{(k)}$ is

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j / (n + \beta)_j. \quad (201)$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \Delta^k (n + \beta)_{k-1}. \quad (202)$$

The model sequence for $\mathcal{M}^{(k)}$ is

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j / (-n - \xi)_j. \quad (203)$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \Delta^k (-n - \xi)_{k-1}. \quad (204)$$

The model sequence for $\mathcal{C}^{(k)}$ is

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j / (\alpha[n + \zeta])_j. \quad (205)$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \Delta^k (\alpha[n + \zeta])_{k-1}. \quad (206)$$

W algorithm: The model sequence for $W^{(k)}$ is

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j t_n^j. \quad (207)$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \square_n^{(k)}[\{\{t_n\}\}]. \tag{208}$$

H transformation: The model sequence for $\mathcal{H}^{(k)}$ is

$$\sigma_n = \sigma + \omega_n \left(\exp(i\alpha n) \sum_{j=0}^{k-1} c_j^+ / (n + \beta)^j + \exp(-i\alpha n) \sum_{j=0}^{k-1} c_j^- / (n + \beta)^j \right). \tag{209}$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \mathcal{P}[P^{(2k)}(\alpha)](n + \beta)^{k-1}. \tag{210}$$

Generalized H transformation: The model sequence for $\mathcal{H}^{(k,m)}$ is

$$\sigma_n = \sigma + \omega_n \sum_{m=1}^M e_m^n \sum_{j=0}^{k-1} c_{m,j} (n + \beta)^{-j}. \tag{211}$$

The annihilation operator is

$$\mathcal{A}_n^{(k)} = \mathcal{P}[P^{(k,m)}(\mathbf{e})](n + \beta)^{k-1}. \tag{212}$$

5.2. Hierarchically consistent iteration

As alternative to the derivation of sequence transformations using model sequences and possibly annihilation operators, one may take some simple sequence transformation T and iterate it k times to obtain a transformation $T^{(k)} = T \circ \dots \circ T$. For the iterated transformation, by construction one has a simple algorithm by construction, but the theoretical analysis is complicated since usually no kernel is known. See for instance the iterated Aitken process where the Δ^2 method plays the role of the simple transformation. However, as is discussed at length in Refs. [36,86], there are usually several possibilities for the iteration. Both problems – unknown kernel and arbitrariness of iteration – are overcome using the concept of hierarchical consistency [36,40,44] that was shown to give rise to powerful algorithms like the \mathcal{J} and the \mathcal{S} transformations [39,40,44]. The basic idea of the concept is to provide a hierarchy of model sequences such that the simple transformation provides a mapping between neighboring levels of the hierarchy. To ensure the latter, normally one has to fix some parameters in the simple transformation to make the iteration consistent with the hierarchy.

A formal description of the concept is given in the following taken mainly from the literature [44]. As an example, the concept is later used to derive the $\mathcal{J}\mathcal{D}$ transformation in Section 5.2.1.

Let $\{\{\sigma_n(\mathbf{c}, \mathbf{p})\}\}_{n=0}^\infty$ be a simple “basic” model sequence that depends on a vector $\mathbf{c} \in \mathbb{K}^a$ of constants, and further parameters \mathbf{p} . Assume that its (anti)limit $\sigma(\mathbf{p})$ exists and is independent of \mathbf{c} . Assume that the basic transformation $T = T(\mathbf{p})$ allows to compute the (anti)limit exactly according to

$$T(\mathbf{p}) : \{\{\sigma_n(\mathbf{c}, \mathbf{p})\}\} \rightarrow \{\{\sigma(\mathbf{p})\}\}. \tag{213}$$

Let the hierarchy of model sequences be given by

$$\{\{\{\sigma_n^{(\ell)}(\mathbf{c}^{(\ell)}, \mathbf{p}^{(\ell)}) | \mathbf{c}^{(\ell)} \in \mathbb{K}^{a^{(\ell)}}\}\}\}_{\ell=0}^L \tag{214}$$

with $a^{(\ell)} > a^{(\ell')}$ for $\ell > \ell'$. Here, ℓ numbers the levels of the hierarchy. Each of the model sequences $\{\{\sigma_n^{(\ell)}(\mathbf{c}^{(\ell)}, \mathbf{p}^{(\ell)})\}\}$ depends on an $a^{(\ell)}$ -dimensional complex vector $\mathbf{c}^{(\ell)}$ and further parameters $\mathbf{p}^{(\ell)}$. Assume that the model sequences of lower levels are also contained in those of higher levels: For all $\ell < L$ and all $\ell' > \ell$ and $\ell' \leq L$, every sequence $\{\{\sigma_n^{(\ell)}(\mathbf{c}^{(\ell)}, \mathbf{p}^{(\ell)})\}\}$ is assumed to be representable as a model sequence $\{\{\sigma_n^{(\ell')}(\mathbf{c}^{(\ell')}, \mathbf{p}^{(\ell')})\}\}$ where $\mathbf{c}^{(\ell')}$ is obtained from $\mathbf{c}^{(\ell)}$ by the natural injection $\mathbb{K}^{a^{(\ell)}} \rightarrow \mathbb{K}^{a^{(\ell')}}$. Assume that for all ℓ with $0 < \ell \leq L$

$$T(\mathbf{p}^{(\ell)}) : \{\{\sigma_n^{(\ell)}(\mathbf{c}^{(\ell)}, \mathbf{p}^{(\ell)})\}\} \rightarrow \{\{\sigma_n^{(\ell-1)}(\mathbf{c}^{(\ell-1)}, \mathbf{p}^{(\ell-1)})\}\} \tag{215}$$

is a mapping between neighboring levels of the hierarchy. Composition yields an iterative transformation

$$T^{(L)} = T(\mathbf{p}^{(0)}) \circ T(\mathbf{p}^{(1)}) \circ \dots \circ T(\mathbf{p}^{(L)}). \tag{216}$$

This transformation is called “hierarchically consistent” or “consistent with the hierarchy”. It maps model sequences $\sigma_n^{(\ell)}(\mathbf{c}^{(\ell)}, \mathbf{p}^{(\ell)})$ to constant sequences if Eq. (213) holds with

$$\{\{\sigma_n^{(0)}(\mathbf{c}^{(0)}, \mathbf{p}^{(0)})\}\} = \{\{\sigma_n(\mathbf{c}, \mathbf{p})\}\}. \tag{217}$$

If instead of Eq. (215) we have

$$T(\mathbf{p}^{(\ell)})(\{\{\sigma_n^{(\ell)}(\mathbf{c}^{(\ell)}, \mathbf{p}^{(\ell)})\}\}) \sim \{\{\sigma_n^{(\ell-1)}(\mathbf{c}^{(\ell-1)}, \mathbf{p}^{(\ell-1)})\}\} \tag{218}$$

for $n \rightarrow \infty$ for all $\ell > 0$ then the iterative transformation $T^{(L)}$ is called “asymptotically consistent with the hierarchy” or “asymptotically hierarchy-consistent”.

5.2.1. Derivation of the $\mathcal{J}\mathcal{D}$ transformation

The simple transformation is the $\mathcal{D}^{(2)}$ transformation

$$s'_n = T(\{\{\omega_n\}\})(\{\{s_n\}\}) = \frac{\Delta^2(s_n/\omega_n)}{\Delta^2(1/\omega_n)} \tag{219}$$

depending on the “parameters” $\{\{\omega_n\}\}$, with basic model sequences

$$\frac{\sigma_n}{\omega_n} = \sigma \frac{1}{\omega_n} + (an + b). \tag{220}$$

The more complicated model sequences of the next level are taken to be

$$\frac{\sigma_n}{\omega_n} = \sigma \frac{1}{\omega_n} + (an + b + (a_1n + b_1)r_n). \tag{221}$$

Application of Δ^2 eliminates the terms involving a and b . The result is

$$\frac{\Delta^2 \sigma_n / \omega_n}{\Delta^2 r_n} = \sigma \frac{\Delta^2 1 / \omega_n}{\Delta^2 r_n} + \left(a_1 n + b_1 + 2a_1 \frac{\Delta r_n}{\Delta^2 r_n} \right) \tag{222}$$

for $\Delta^2 r_n \neq 0$. Assuming that for large n

$$\frac{\Delta r_n}{\Delta^2 r_n} = An + B + o(1) \tag{223}$$

holds, the result is asymptotically of the same form as the model sequence in Eq. (220), namely

$$\frac{\sigma'_n}{\omega'_n} = \sigma \frac{1}{\omega'_n} + (a'n + b' + o(1)) \tag{224}$$

with renormalized “parameters”

$$1/\omega'_n = \frac{\Delta^2(1/\omega_n)}{\Delta^2 r_n} \tag{225}$$

and obvious identifications for a' and b' .

We now assume that this mapping between two neighboring levels of the hierarchy can be extended to any two neighboring levels, provided that one introduces ℓ -dependent quantities, especially $r_n \rightarrow r_n^{(\ell)}$ with $\zeta_n^{(\ell)} = \Delta^2 r_n^{(\ell)} \neq 0$, $s_n/\omega_n \rightarrow N_n^{(\ell)}$, $1/\omega_n \rightarrow D_n^{(\ell)}$ and $s'_n/\omega'_n \rightarrow N_n^{(\ell+1)}$, $1/\omega'_n \rightarrow D_n^{(\ell+1)}$.

Iterating in this way leads to algorithm (151).

Condition (223) or more generally

$$\frac{\Delta r_n^{(\ell)}}{\Delta^2 r_n^{(\ell)}} = A_\ell n + B_\ell + o(1) \tag{226}$$

for given ℓ and for large n is satisfied in many cases. For instance, it is satisfied if there are constants $\beta_\ell \neq 0$, γ_ℓ and $\delta_\ell \neq 0$ such that

$$\Delta r_n^{(\ell)} \sim \beta_\ell \begin{cases} \left(\frac{\delta_\ell + 1}{\delta_\ell} \right)^n & \text{for } \gamma_\ell = 0, \\ \left(\frac{\delta_\ell + 1}{\gamma_\ell} \right)_n / \left(\frac{\delta_\ell}{\gamma_\ell} \right)_n & \text{otherwise.} \end{cases} \tag{227}$$

This is for instance the case for $r_n^{(\ell)} = n^{\zeta_\ell}$ with $\zeta_\ell(\zeta_\ell - 1) \neq 0$.

The kernel of $\mathcal{J}\mathcal{D}^{(k)}$ may be found inductively in the following way:

$$\begin{aligned} N_n^{(k)} - \sigma D_n^{(k)} &= 0 \\ \Rightarrow \Delta^2(N_n^{(k-1)} - \sigma D_n^{(k-1)}) &= 0 \\ \Rightarrow N_n^{(k-1)} - \sigma D_n^{(k-1)} &= a_{k-1}n + b_{k-1} \\ \Rightarrow \Delta^2(N_n^{(k-2)} - \sigma D_n^{(k-2)}) &= (a_{k-1}n + b_{k-1})\zeta_n^{(k-2)} \\ \Rightarrow N_n^{(k-2)} - \sigma D_n^{(k-2)} &= a_{k-2}n + b_{k-2} + \sum_{j=0}^{n-2} \sum_{n'=0}^j (a_{k-1}n' + b_{k-1})\zeta_{n'}^{(k-2)} \end{aligned} \tag{228}$$

yielding the result

$$\begin{aligned}
 N_n^{(0)} - \sigma D_n^{(0)} = & a_0 n + b_0 + \sum_{j=0}^{n-2} \sum_{n_1=0}^j \zeta_{n_1}^{(0)} (a_1 n_1 + b_1 + \dots \\
 & + (a_{k-2} n + b_{k-2} + \sum_{j_{k-2}=0}^{n_{k-2}-2} \sum_{n_{k-1}=0}^{j_{k-2}} \zeta_{n_{k-1}}^{(k-2)} (a_{k-1} n_{k-1} + b_{k-1})) \Big). \tag{229}
 \end{aligned}$$

Here, the definitions $N_n^{(0)} = \sigma_n / \omega_n$ and $D_n^{(0)} = 1 / \omega_n$ may be used to obtain the model sequence $\{\{\sigma_n\}\}$ for $\mathcal{J}\mathcal{D}^{(k)}$, that may be identified as kernel of that transformation, and also may be regarded as model sequence of the k th level according to $\{\{\sigma_n^{(k)}(\mathbf{c}^{(k)}, \mathbf{p}^{(k)})\}\}$ with $\mathbf{c}^{(k)} = (a_0, b_0, \dots, a_{k-1}, b_{k-1})$ and $\mathbf{p}^{(k)}$ corresponds to $\omega_n^{(k)} = 1 / D_n^{(k)}$ and the $\{\zeta_n^{(\kappa)} \mid 0 \leq \kappa \leq k - 2\}$.

We note this as a theorem:

Theorem 2. *The kernel of $\mathcal{J}\mathcal{D}^{(k)}$ is given by the set of sequences $\{\{\sigma_n\}\}$ such that Eq. (229) holds with $N_n^{(0)} = \sigma_n / \omega_n$ and $D_n^{(0)} = 1 / \omega_n$.*

5.2.2. Important special cases

Here, we give the hierarchies of model sequences for sequence transformations derived via hierarchically consistent iteration.

J transformation: The most prominent example is the \mathcal{J} transformation (actually a large class of transformations). The corresponding hierarchy of model sequences provided by the kernels that are explicitly known according to the following theorem:

Theorem 3 (Homeier [36]). *The kernel of the $\mathcal{J}^{(k)}$ transformation is given by the sequences $\{\{\sigma_n\}\}$ with elements of the form*

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k-1} c_j \psi_j(n) \tag{230}$$

with

$$\begin{aligned}
 \psi_0(n) &= 1, \\
 \psi_1(n) &= \sum_{n_1=0}^{n-1} \delta_{n_1}^{(0)}, \\
 \psi_2(n) &= \sum_{n_1=0}^{n-1} \delta_{n_1}^{(0)} \sum_{n_2=0}^{n_1-1} \delta_{n_2}^{(1)}, \\
 &\vdots \\
 \psi_{k-1}(n) &= \sum_{n > n_1 > n_2 > \dots > n_{k-1}} \delta_{n_1}^{(0)} \delta_{n_2}^{(1)} \dots \delta_{n_{k-1}}^{(k-2)}
 \end{aligned} \tag{231}$$

with arbitrary constants c_0, \dots, c_{k-1} .

\mathcal{I} transformation: Since the \mathcal{I} transformation is a special case of the \mathcal{J} transformation (cf. Table 1) and [44], its kernels (corresponding to the hierarchy of model sequences) are explicitly known according to the following theorem:

Theorem 4 (Homeier [44, Theorem 8]). *The kernel of the $\mathcal{J}^{(k)}$ transformation is given by the sequences $\{\{\sigma_n\}\}$ with elements of the form*

$$\begin{aligned} \sigma_n = & \sigma + \exp(-i\alpha n)\omega_n \left[d_0 + d_1 \exp(2i\alpha n) \right. \\ & + \sum_{n_1=0}^{n-1} \sum_{n_2=0}^{n_1-1} \exp(2i\alpha(n_1 - n_2))(d_2 + d_3 \exp(2i\alpha n_2))\Delta_{n_2}^{(0)} + \dots \\ & + \sum_{n > n_1 > n_2 > \dots > n_{2k-2}} \exp(2i\alpha[n_1 - n_2 + \dots + n_{2k-3} - n_{2k-2}]) \\ & \left. (d_{2k-2} + d_{2k-1} \exp(2i\alpha n_{2k-2})) \prod_{j=0}^{k-2} \Delta_{n_{2j+2}}^{(j)} \right] \end{aligned} \quad (232)$$

with constants d_0, \dots, d_{2k-1} . Thus, we have $s = \mathcal{J}_n^{(k')}(\alpha, \{\{s_n\}\}, \{\{\omega_n\}\}, \{\Delta_n^{(k)}\})$ for $k' \geq k$ for sequences of this form.

5.3. A two-step approach

In favorable cases, one may use a two-step approach for the construction of sequence transformations:

Step 1: Use asymptotic analysis of the remainder $R_n = s_n - s$ of the given problem to find the adequate model sequence (or hierarchy of model sequences) for large n .

Step 2: Use the methods described in Sections 5.1 or 5.2 to construct the sequence transformation adapted to the problem.

This is, of course, a mathematically promising approach. A good example for the two-step approach is the derivation of the $d^{(m)}$ transformations by Levin and Sidi [54] (cf. also Section 3.2).

But there are two difficulties with this approach.

The first difficulty is a practical one. In many cases, the problems to be treated in applications are simply too complicated to allow to perform Step 1 of the two-step approach.

The second difficulty is a more mathematical one. The optimal system of functions $f_j(n)$ used in the asymptotic expansion

$$s_n - s \sim \sum_{j=0}^{\infty} c_j f_j(n) \quad (233)$$

with $f_{j+1}(n) = o(f_j(n))$, i.e., the optimal *asymptotic scale* [102, p. 2], is not clear a priori. For instance, as the work of Weniger has shown, sequence transformations like the Levin transformation that are based on expansions in powers of $1/n$, i.e., the asymptotic scale $\phi_j(n) = 1/(n + \beta)^j$, are not always superior to, and even often worse than those based upon factorial series, like Weniger's \mathcal{S}

transformation that is based on the asymptotic scale $\psi_f(n) = 1/(n + \beta)_j$. To find an optimal asymptotic scale in combination with nonlinear sequence transformations seems to be an open mathematical problem.

Certainly, the proper choice of remainder estimates [50] is also crucial in the context of Levin-type sequence transformations. See also Section 9.

6. Properties of Levin-type transformations

6.1. Basic properties

Directly from the definition in Eqs. (65) and (66), we obtain the following theorem. The proof is left to the interested reader.

Theorem 5. Any Levin-type sequence transformation \mathcal{T} is quasilinear, i.e., we have

$$\mathcal{T}_n^{(k)}(\{\{As_n + B\}\}, \{\{\omega_n\}\}) = A\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) + B \quad (234)$$

for arbitrary constants A and B . It is multiplicatively invariant in ω_n , i.e., we have

$$\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{C\omega_n\}\}) = \mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) \quad (235)$$

for arbitrary constants $C \neq 0$.

For a coefficient set A define the sets $Y_n^{(k)}[A]$ by

$$Y_n^{(k)}[A] = \left\{ (x_0, \dots, x_k) \in \mathbb{F}^{k+1} \mid \sum_{j=0}^k \lambda_{n,j}^{(k)} x_j \neq 0 \right\}. \quad (236)$$

Since $\mathcal{T}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\})$ for given coefficient set A depends only on the $2k+2$ numbers s_n, \dots, s_{n+k} and $\omega_n, \dots, \omega_{n+k}$, it may be regarded as a mapping

$$U_n^{(k)} : \mathbb{C}^{k+1} \times Y_n^{(k)}[A] \Rightarrow \mathbb{C}, \quad (x, y) \mapsto U_n^{(k)}(x | y) \quad (237)$$

such that

$$\mathcal{T}_n^{(k)} = U_n^{(k)}(s_n, \dots, s_{n+k} | \omega_n, \dots, \omega_{n+k}). \quad (238)$$

The following theorem is a generalization of theorems for the \mathcal{J} transformation [36, Theorem 5] and the \mathcal{S} transformation [44, Theorem 5].

Theorem 6. (I–0) The $\mathcal{T}^{(k)}$ transformation can be regarded as continuous mapping $U_n^{(k)}$ on $\mathbb{C}^{k+1} \times Y_n^{(k)}[A]$ where $Y_n^{(k)}[A]$ is defined in Eq. (236):

(I–1) According to Theorem 5, $U_n^{(k)}$ is a homogeneous function of first degree in the first $(k+1)$ variables and a homogeneous function of degree zero in the last $(k+1)$ variables. Hence, for all vectors $\mathbf{x} \in \mathbb{C}^{k+1}$ and $\mathbf{y} \in Y_n^{(k)}[A]$ and for all complex constants s and $t \neq 0$ the equations

$$\begin{aligned} U_n^{(k)}(s\mathbf{x} | \mathbf{y}) &= sU_n^{(k)}(\mathbf{x} | \mathbf{y}), \\ U_n^{(k)}(\mathbf{x} | t\mathbf{y}) &= U_n^{(k)}(\mathbf{x} | \mathbf{y}) \end{aligned} \quad (239)$$

hold.
 (I – 2) $U_n^{(k)}$ is linear in the first $(k + 1)$ variables. Thus, for all vectors $\mathbf{x} \in \mathbb{C}^{k+1}$, $\mathbf{x}' \in \mathbb{C}^{k+1}$, und $\mathbf{y} \in Y_n^{(k)}[A]$

$$U_n^{(k)}(\mathbf{x} + \mathbf{x}' | \mathbf{y}) = U_n^{(k)}(\mathbf{x} | \mathbf{y}) + U_n^{(k)}(\mathbf{x}' | \mathbf{y}) \tag{240}$$

holds.
 (I – 3) For all constant vectors $\mathbf{c} = (c, c, \dots, c) \in \mathbb{C}^{k+1}$ and all vectors $\mathbf{y} \in Y_n^{(k)}[A]$ we have

$$U_n^{(k)}(\mathbf{c} | \mathbf{y}) = c. \tag{241}$$

Proof. These are immediate consequences of the definitions. \square

6.2. The limiting transformation

We note that if a limiting transformation $\overset{\circ}{\mathcal{F}}[\overset{\circ}{A}]$ exists, it is also of Levin-type, and thus, the above theorems apply to the limiting transformation as well.

Also, we have the following result for the kernel of the limiting transformation:

Theorem 7. *Suppose that for a Levin-type sequence transformation $\mathcal{F}^{(k)}$ of order k there exists a limiting transformation $\overset{\circ}{\mathcal{F}}^{(k)}$ with characteristic polynomial $\overset{\circ}{\Pi} \in \mathbb{P}^k$ given by*

$$\overset{\circ}{\Pi}^{(k)}(z) = \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} z^j = \prod_{\ell=1}^M (z - \zeta_{\ell})^{m_{\ell}}, \tag{242}$$

where the zeroes $\zeta_{\ell} \neq 0$ have multiplicities m_{ℓ} . Then the kernel of the limiting transformation consists of all sequences $\{\{s_n\}\}$ with elements of the form

$$\sigma_n = \sigma + \omega_n \sum_{\ell=1}^M \zeta_{\ell}^n P_{\ell}(n), \tag{243}$$

where $P_{\ell} \in \mathbb{P}^{m_{\ell}-1}$ are arbitrary polynomials and $\{\{\omega_n\}\} \in \overset{\circ}{\mathbb{Y}}^{(k)}$.

Proof. This follows directly from the observation that for such sequences $(\sigma_n - \sigma)/\omega_n$ is nothing but a finite linear combination of the solutions $\varphi_{n,\ell,j_{\ell}}^{(k)} = n^{j_{\ell}} \zeta_{\ell}^n$ with $\ell = 1, \dots, M$ and $j_{\ell} = 0, \dots, m_{\ell} - 1$ of the recursion relation

$$\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} v_{n+j} = 0 \tag{244}$$

and thus, it is annihilated by $\mathcal{P}[\overset{\circ}{\Pi}^{(k)}]$. \square

6.3. Application to power series

Here, we generalize some results of Weniger [88] that regard the application of Levin-type sequence transformations to power series.

We use the definitions in Eq. (27). Like Padé approximants, Levin-type sequence transformations yield rational approximants when applied to the partial sums $f_n(z)$ of a power series $f(z)$ with terms $a_j = c_j z^j$. These approximations offer a practical way for the analytical continuation of power series to regions outside of their circle of convergence. Furthermore, the poles of the rational approximations model the singularities of $f(z)$. They may also be used to approximate further terms beyond the last one used in constructing the rational approximant.

When applying a Levin-type sequence transformation \mathcal{T} to a power series, remainder estimates $\omega_n = m_n z^{\gamma+n}$ will be used. We note that t variants correspond to $m_n = c_n$, $\gamma = 0$, u variants correspond to $m_n = c_n(n + \beta)$, $\gamma = 0$, \tilde{t} variants to $m_n = c_{n+1}$, $\gamma = 1$. Thus, for these variants, m_n is independent of z (Case A). For v variants, we have $m_n = c_{n+1}c_n/(c_n - c_{n+1}z)$, and $\gamma = 1$. In this case, $1/m_n \in \mathbb{P}^{(1)}$ is a linear function of z (Case B).

Application of \mathcal{T} yields after some simplification

$$\mathcal{T}_n^{(k)}(\{\{f_n(z)\}\}, \{\{m_n z^{\gamma+n}\}\}) = \frac{\sum_{\ell=0}^{n+k} z^\ell \sum_{j=\max(0, k-\ell)}^k (\lambda_{n,j}^{(k)} / m_{n+j}) c_{\ell-(k-j)}}{\sum_{j=0}^k (\lambda_{n,j}^{(k)} / m_{n+j}) z^{k-j}} = \frac{P_n^{(k)}[T](z)}{Q_n^{(k)}[T](z)}, \tag{245}$$

where in Case A, we have $P_n^{(k)}[T] \in \mathbb{P}^{n+k}$, $Q_n^{(k)}[T] \in \mathbb{P}^k$, and in Case B, we have $P_n^{(k)}[T] \in \mathbb{P}^{n+k+1}$, $Q_n^{(k)}[T] \in \mathbb{P}^{k+1}$. One needs the $k + 1 + \gamma$ partial sums $f_n(z), \dots, f_{n+k+\gamma}(z)$ to compute these rational approximants. This should be compared to the fact that for the computation of the Padé approximant $[n + k + \gamma/k + \gamma]$ one needs the $2k + 2\gamma + 1$ partial sums $f_n(z), \dots, f_{n+2k+2\gamma}(z)$.

We show that Taylor expansion of these rational approximants reproduces all terms of power series that have been used to calculate the rational approximation.

Theorem 8. *We have*

$$\mathcal{T}_n^{(k)}(\{\{f_n(z)\}\}, \{\{m_n z^{\gamma+n}\}\}) - f(z) = O(z^{n+k+1+\tau}), \tag{246}$$

where $\tau=0$ for t and u variants corresponding to $m_n=c_n$, $\gamma=0$, or $m_n=c_n(n+\beta)$, $\gamma=0$, respectively, while $\tau=1$ holds for the v variant corresponding to $m_n=c_{n+1}c_n/(c_n-c_{n+1}z)$, $\gamma=1$, and for the \tilde{t} variants corresponding to $m_n=c_{n+1}$, $\gamma=1$, one obtains $\tau=1$ if \mathcal{T} is convex.

Proof. Using the identity

$$\mathcal{T}_n^{(k)}(\{\{f_n(z)\}\}, \{\{m_n z^{\gamma+n}\}\}) = f(z) + \mathcal{T}_n^{(k)}(\{\{f_n(z) - f(z)\}\}, \{\{m_n z^{\gamma+n}\}\}) \tag{247}$$

that follows from Theorem 5, we obtain after some easy algebra

$$\mathcal{T}_n^{(k)}(\{\{f_n(z)\}\}, \{\{m_n z^{\gamma+n}\}\}) - f(z) = z^{n+k+1} \frac{\sum_{\ell=0}^{\infty} z^\ell \sum_{j=0}^k (\lambda_{n,j}^{(k)} / m_{n+j}) c_{\ell+n+j+1}}{\sum_{j=0}^k (\lambda_{n,j}^{(k)} / m_{n+j}) z^{k-j}}. \tag{248}$$

This shows that the right-hand side is at least $O(z^{n+k+1})$ since the denominator is $O(1)$ due to $\lambda_{n,k}^{(k)} \neq 0$. For the \tilde{t} variant, the term corresponding to $\ell = 0$ in the numerator is $\sum_{j=0}^k \lambda_{n,j}^{(k)} = \Pi_n^{(k)}(1)$ that vanishes for convex \mathcal{T} . For the v variant, that term is $\sum_{j=0}^k \lambda_{n,j}^{(k)} (c_{n+j} - c_{n+j+1}z) / c_{n+j}$ that simplifies to $(-z) \sum_{j=0}^k \lambda_{n,j}^{(k)} c_{n+j+1} / c_{n+j}$ for convex \mathcal{T} . This finishes the proof. \square

7. Convergence acceleration results for Levin-type transformations

7.1. General results

We note that Germain-Bonne [23] developed a theory of the regularity and convergence acceleration properties of sequence transformations that was later extended by Weniger [84, Section 12; 88, Section 6] to sequence transformations that depend explicitly on n and on an auxiliary sequence of remainder estimates. The essential results of this theory apply to convergence acceleration of linearly convergent sequences. Of course, this theory can be applied to Levin-type sequence transformations. However, for the latter transformations, many results can be obtained more easily and also, one may obtain results of a general nature that are also applicable to other convergence types like logarithmic convergence. Thus, we are not going to use the Germain–Bonne–Weniger theory in the present article.

Here, we present some general convergence acceleration results for Levin-type sequence transformations that have a limiting transformation. The results, however, do not completely determine which transformation provides the best extrapolation results for a given problem sequence since the results are asymptotic in nature, but in practice, one is interested in obtaining good extrapolation results from as few members of the problem sequence as possible. Thus, it may well be that transformations with the same asymptotic behavior of the results perform rather differently in practice.

Nevertheless, the results presented below provide a first indication which results one may expect for large classes of Levin-type sequence transformations.

First, we present some results that show that the limiting transformation essentially determines for which sequences Levin-type sequence transformations are accelerative. The speed of convergence will be analyzed later.

Theorem 9. *Assume that the following asymptotic relations hold for large n :*

$$\lambda_{n,j}^{(k)} \sim \overset{\circ}{\lambda}_j^{(k)}, \quad \overset{\circ}{\lambda}_k^{(k)} \neq 0, \tag{249}$$

$$\frac{s_n - s}{\omega_n} \sim \sum_{v=1}^A c_v \zeta_v^n, \quad c_v \zeta_v \neq 0, \quad \overset{\circ}{\Pi}^{(k)}(\zeta_v) = 0, \tag{250}$$

$$\frac{\omega_{n+1}}{\omega_n} \sim \rho \neq 0, \quad \overset{\circ}{\Pi}^{(k)}(1/\rho) \neq 0. \tag{251}$$

Then, $\{\{\mathcal{F}_n^{(k)}\}\}$ accelerates $\{s_n\}$ to s , i.e., we have

$$\lim_{n \rightarrow \infty} \frac{\mathcal{F}_n^{(k)} - s}{s_n - s} = 0. \tag{252}$$

Proof. Rewriting

$$\frac{\mathcal{F}_n^{(k)} - s}{s_n - s} = \frac{\omega_n}{s_n - s} \frac{\sum_{j=0}^k \lambda_{n,j}^{(k)} (s_{n+j} - s) / \omega_{n+j}}{\sum_{j=0}^k \lambda_{n,j}^{(k)} \omega_n / \omega_{n+j}}. \tag{253}$$

one may perform the limit for $n \rightarrow \infty$ upon using the assumptions according to

$$\frac{\mathcal{F}_n^{(k)} - s}{s_n - s} \rightarrow \frac{\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \sum_v c_v \zeta_v^{n+j}}{\sum_v c_v \zeta_v^n \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \rho^{-j}} = \frac{\sum_v c_v \zeta_v^n \overset{\circ}{\Pi}^{(k)}(\zeta_v)}{\overset{\circ}{\Pi}^{(k)}(1/\rho) \sum_v c_v \zeta_v^n} = 0 \tag{254}$$

since $\omega_n/\omega_{n+j} \rightarrow \rho^{-j}$. \square

Thus, the zeroes ζ_v of the characteristic polynomial of the limiting transformation are of particular importance.

It should be noted that the above assumptions correspond to a more complicated convergence type than linear or logarithmic convergence if $|\zeta_1| = |\zeta_2| \geq |\zeta_3| \geq \dots$. This is the case, for instance, for the $\mathcal{H}^{(k)}$ transformation where the limiting transformation has the characteristic polynomial $P^{(2k)}(\alpha)$ with k -fold zeroes at $\exp(i\alpha)$ and $\exp(-i\alpha)$. Another example is the $\mathcal{F}^{(k)}$ transformation where the limiting transformation has characteristic polynomials $Q^{(2k)}(\alpha)$ with zeroes at $\exp(\pm i\alpha)/\Theta_j$, $j = 0, \dots, k - 1$.

Specializing to $A = 1$ in Theorem 9, we obtain the following corollary:

Corollary 10. *Assume that the following asymptotic relations hold for large n :*

$$\lambda_{n,j}^{(k)} \sim \overset{\circ}{\lambda}_j^{(k)}, \quad \overset{\circ}{\lambda}_k^{(k)} \neq 0, \tag{255}$$

$$\frac{s_n - s}{\omega_n} \sim cq^n, \quad cq \neq 0, \quad \overset{\circ}{\Pi}^{(k)}(q) = 0, \tag{256}$$

$$\frac{\omega_{n+1}}{\omega_n} \sim \rho \neq 0, \quad \overset{\circ}{\Pi}^{(k)}(1/\rho) \neq 0. \tag{257}$$

Then, $\{\{\mathcal{F}_n^{(k)}\}\}$ accelerates $\{s_n\}$ to s , i.e., we have

$$\lim_{n \rightarrow \infty} \frac{\mathcal{F}_n^{(k)} - s}{s_n - s} = 0. \tag{258}$$

Note that the assumptions of Corollary 10 imply

$$\frac{s_{n+1} - s}{s_n - s} = \frac{s_{n+1} - s}{\omega_{n+1}} \frac{\omega_n}{s_n - s} \frac{\omega_{n+1}}{\omega_n} \sim \rho \frac{cq^{n+1}}{cq^n} = \rho q \tag{259}$$

and thus, Corollary 10 corresponds to linear convergence for $0 < |\rho q| < 1$ and to logarithmic convergence for $\rho q = 1$.

Many important sequence transformations have convex limiting transformations, i.e., the characteristic polynomials satisfy $\overset{\circ}{\Pi}^{(k)}(1) = 0$. In this case, they accelerate linear convergence. More exactly, we have the following corollary:

Corollary 11. *Assume that the following asymptotic relations hold for large n :*

$$\lambda_{n,j}^{(k)} \sim \overset{\circ}{\lambda}_j^{(k)}, \quad \overset{\circ}{\lambda}_k^{(k)} \neq 0, \tag{260}$$

$$\frac{s_n - s}{\omega_n} \sim c, \quad c \neq 0, \quad \overset{\circ}{\Pi}^{(k)}(1) = 0, \tag{261}$$

$$\frac{\omega_{n+1}}{\omega_n} \sim \rho \neq 0, \quad \mathring{\Pi}^{(k)}(1/\rho) \neq 0. \tag{262}$$

Then, $\{\{\mathcal{F}_n^{(k)}\}\}$ accelerates $\{\{s_n\}\}$ to s , i.e., we have

$$\lim_{n \rightarrow \infty} \frac{\mathcal{F}_n^{(k)} - s}{s_n - s} = 0. \tag{263}$$

Hence, any Levin-type sequence transformation with a convex limiting transformation accelerates linearly convergent sequences with

$$\lim_{n \rightarrow \infty} \frac{s_{n+1} - s}{s_n - s} = \rho, \quad 0 < |\rho| < 1 \tag{264}$$

such that $\mathring{\Pi}^{(k)}(1/\rho) \neq 0$ for suitably chosen remainder estimates ω_n satisfying $(s_n - s)/\omega_n \rightarrow c \neq 0$.

Proof. Specializing Corollary 10 to $q = 1$, it suffices to prove the last assertion. Here, the proof follows from the observation that $(s_{n+1} - s)/(s_n - s) \sim \rho$ and $(s_n - s)/\omega_n \sim c$ imply $\omega_{n+1}/\omega_n \sim \rho$ for large n in view of the assumptions. \square

Note that Corollary 11 applies for instance to suitable variants of the Levin transformation, the ${}_p\mathbf{J}$ transformation and, more generally, of the \mathcal{J} transformation. In particular, it applies to t, \tilde{t}, u and v variants, since in the case of linear convergence, one has $\Delta s_n/\Delta s_{n-1} \sim \rho$ which entails $(s_n - s)/\omega_n \sim c$ for all these variants by simple algebra.

Now, some results for the speed of convergence are given. Matos [59] presented convergence theorems for sequence transformations based on annihilation difference operators with characteristic polynomials with constants coefficients that are close in spirit to the theorems given below. However, it should be noted that the theorems presented here apply to large classes of Levin-type transformations that have a limiting transformation (the latter, of course, has a characteristic polynomial with constants coefficients).

Theorem 12. (C-1) *Suppose that for a Levin-type sequence transformation $\mathcal{F}^{(k)}$ of order k there is a limiting transformation $\mathring{\mathcal{F}}^{(k)}$ with characteristic polynomial $\mathring{\Pi} \in \mathbb{P}^k$ given by Eq. (242) where the multiplicities m_ℓ of the zeroes $\zeta_\ell \neq 0$ satisfy $m_1 \leq m_2 \leq \dots \leq m_M$. Let*

$$\lambda_{n,j}^{(k)} \frac{n^{m_1-1}}{(n+j)^{m_1-1}} \sim \mathring{\lambda}_j^{(k)} \left(\sum_{t=0}^{\infty} \frac{e_t^{(k)}}{(n+j)^t} \right), \quad e_0^{(k)} = 1 \tag{265}$$

for $n \rightarrow \infty$.

(C-2) *Assume that $\{\{s_n\}\} \in \mathbb{S}^{\mathbb{K}}$ and $\{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}}$. Assume further that for $n \rightarrow \infty$ the asymptotic expansion*

$$\frac{s_n - s}{\omega_n} \sim \sum_{\ell=1}^M \zeta_\ell^n \sum_{r=0}^{\infty} c_{\ell,r} n^{-r} \tag{266}$$

holds, and put

$$r_\ell = \min\{r \in \mathbb{N}_0 \mid f_{\ell,r+m_1} \neq 0\}, \tag{267}$$

where

$$f_{\ell,v} = \sum_{r=0}^v e_{v-r}^{(k)} c_{\ell,r} \tag{268}$$

and

$$B_{\ell} = (-1)^{m_{\ell}} \frac{d^{m_{\ell}} \overset{\circ}{\Pi}^{(k)}}{dx^{m_{\ell}}}(\zeta_{\ell}) \tag{269}$$

for $\ell = 1, \dots, M$.

(C-3) Assume that the following limit exists and satisfies

$$0 \neq \lim_{n \rightarrow \infty} \frac{\omega_{n+1}}{\omega_n} = \rho \notin \{\zeta_{\ell}^{-1} \mid \ell = 1, \dots, M\}. \tag{270}$$

Then we have

$$\frac{\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) - s}{\omega_n} \sim \frac{\sum_{\ell=1}^M f_{\ell, r_{\ell} + m_{\ell}} \zeta_{\ell}^{n+m_{\ell}} \binom{r_{\ell} + m_{\ell}}{r_{\ell}} B_{\ell} / n^{r_{\ell} + m_{\ell} - m_1}}{\overset{\circ}{\Pi}^{(k)}(1/\rho)} \frac{1}{n^{2m_1}}. \tag{271}$$

Thus, $\{\{\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\})\}\}$ accelerates $\{\{s_n\}\}$ to s at least with order $2m_1$, i.e.,

$$\frac{\mathcal{F}_n^{(k)} - s}{s_n - s} = O(n^{-2m_1 - \tau}), \quad \tau \geq 0 \tag{272}$$

if $c_{\ell,0} \neq 0$ for all ℓ .

Proof. We rewrite $\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) = \mathcal{F}_n^{(k)}$ as defined in Eq. (11) in the form

$$\mathcal{F}_n^{(k)} - s = \omega_n \frac{\sum_{j=0}^k \lambda_{n,j}^{(k)} (s_{n+j} - s) / \omega_{n+j}}{\sum_{j=0}^k \lambda_{n,j}^{(k)} \omega_n / \omega_{n+j}} \sim \omega_n \frac{\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \sum_{t=0}^{\infty} \frac{e_j^{(k)} (n+j)^{m_1-1} \frac{s_{n+j}-s}{\omega_{n+j}}}{(n+j)^t n^{m_1-1}}}{\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \frac{1}{\rho^j}} \tag{273}$$

for large n where we used Eq. (265) in the numerator, and in the denominator the relation $\omega_n / \omega_{n+j} \rightarrow \rho^{-j}$ that follows by repeated application of Eq. (270). Insertion of (266) now yields

$$\mathcal{F}_n^{(k)} - s \sim \frac{\omega_n}{n^{m_1-1} \overset{\circ}{\Pi}^{(k)}(1/\rho)} \sum_{\ell=1}^M \sum_{r=0}^{\infty} f_{\ell, r+m_1} \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \frac{\zeta_{\ell}^{n+j}}{(n+j)^{r+1}}, \tag{274}$$

where Eq. (268) was used. Also the fact was used that $\mathcal{P}[\overset{\circ}{\Pi}^{(k)}]$ annihilates any linear combination of the solutions $\varphi_{n,\ell,j}^{(k)} = n^{j_{\ell}} \zeta_{\ell}^n$ with $\ell = 1, \dots, M$ and $j_{\ell} = 0, \dots, m_1 - 1$ of the recursion relation (244) since each ζ_{ℓ} is a zero with multiplicity exceeding $m_1 - 1$. Invoking Lemma C.1 given in Appendix C one obtains

$$\mathcal{F}_n^{(k)} - s \sim \frac{\omega_n}{n^{m_1-1} \overset{\circ}{\Pi}^{(k)}(1/\rho)} \sum_{\ell=1}^M \sum_{r=0}^{\infty} f_{\ell, r+m_1} \zeta_{\ell}^{n+m_{\ell}} \binom{r+m_{\ell}}{r} \frac{(-1)^{m_{\ell}} d^{m_{\ell}} \overset{\circ}{\Pi}^{(k)}}{n^{r+m_{\ell}+1} dx^{m_{\ell}}}(\zeta_{\ell}). \tag{275}$$

The proof of Eq. (271) is completed taking leading terms in the sums over r . Since $s_n - s \sim \omega_n Z^n \sum_{\ell \in I} (\zeta_{\ell} / Z)^n c_{\ell,0}$ where $Z = \max\{|\zeta_{\ell}| \mid \ell = 1, \dots, M\}$, and $I = \{\ell = 1, \dots, M \mid Z = |\zeta_{\ell}|\}$, Eq. (272) is obtained where $\tau = \min\{r_{\ell} + m_{\ell} - m_1 \mid \ell \in I\}$. \square

If $\omega_{n+1}/\omega_n \sim \rho$, where $\mathring{\Pi}^{(k)}(1/\rho) = 0$, i.e., if (C-3) of Theorem 12 does not hold, then the denominators vanish asymptotically. In this case, one has to investigate whether the numerators or the denominators vanish faster.

Theorem 13. *Assume that (C-1) and (C-2) of Theorem 12 hold.*

(C-3') *Assume that for $n \rightarrow \infty$ the asymptotic relation*

$$\frac{\omega_{n+1}}{\omega_n} \sim \rho \exp(\varepsilon_n), \quad \rho \neq 0 \tag{276}$$

holds where

$$\frac{1}{\lambda!} \frac{d^\lambda \mathring{\Pi}^{(k)}(1/\rho)}{dx^\lambda} = \begin{cases} 0 & \text{for } \lambda = 0, \dots, \mu - 1 \\ C \neq 0 & \text{for } \lambda = \mu \end{cases} \tag{277}$$

and

$$\varepsilon_n \rightarrow 0, \quad \frac{\varepsilon_{n+1}}{\varepsilon_n} \rightarrow 1 \tag{278}$$

for large n . Define δ_n via $\exp(-\varepsilon_n) = 1 + \delta_n \rho$.

Then we have for large n

$$\frac{\mathcal{F}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}) - s}{\omega_n} \sim \frac{\sum_{\ell=1}^M f_{\ell, r_\ell + m_1} \zeta_\ell^{n+m_\ell} \binom{r_\ell + m_\ell}{r_\ell} B_\ell / n^{r_\ell + m_\ell - m_1}}{C(\delta_n)^\mu} \frac{1}{n^{2m_1}}. \tag{279}$$

Proof. The proof proceeds as the proof of Theorem 12 but in the denominator we use

$$\sum_{j=0}^k \lambda_{n,j}^{(k)} \frac{\omega_n}{\omega_{n+j}} \sim C(\delta_n)^\mu \tag{280}$$

that follows from Lemma C.2 given in Appendix C. \square

Thus, the effect of the sequence transformation in this case essentially depends on the question whether $(\delta_n)^{-\mu} n^{-2m_1}$ goes to 0 for large n or not. In many important cases like the Levin transformation and the $p\mathbf{J}$ transformations, we have $M = 1$ and $m_1 = k$. We note that Theorem 11 becomes especially important in the case of logarithmic convergence since for instance for $M = 1$ one observes that $(s_{n+1} - s)/(s_n - s) \sim 1$ and $(s_n - s)/\omega_n \sim \zeta_1^n c_{1,0} \neq 0$ imply $\omega_{n+1}/\omega_n \sim 1/\zeta_1$ for large n such that the denominators vanish asymptotically. In this case, we have $\mu = m_1$ whence $(\delta_n)^{-\mu} n^{-2m_1} = O(n^{-m_1})$ if $\delta_n = O(1/n)$. This reduction of the speed of convergence of the acceleration process from $O(n^{-2k})$ to $O(n^{-k})$ in the case of logarithmic convergence is a generic behavior that is reflected in a number of theorems regarding convergence acceleration properties of Levin-type sequence transformations. Examples are Sidi's theorem for the Levin transformation given below (Theorem 15), and for the $p\mathbf{J}$ transformation the Corollaries 18 and 19 given below, cf. also [84, Theorems 13.5, 13.9, 13.11, 13.12, 14.2].

The following theorem was given by Matos [59] where the proof may be found. To formulate it, we define that a sequence $\{\{u_n\}\}$ has *property M* if it satisfies

$$\frac{u_{n+1}}{u_n} \sim 1 + \frac{\alpha}{n} + r_n \quad \text{with } r_n = o(1/n), \quad \Delta^\ell r_n = o(\Delta^\ell(1/n)) \quad \text{for } n \rightarrow \infty. \tag{281}$$

Theorem 14 (Matos [59, Theorem 13]). *Let $\{\{s_n\}\}$ be a sequence such that*

$$s_n - s = \omega_n(a_1g_1^{(1)}(n) + \dots + a_kg_1^{(k)}(n) + \rho_n) \tag{282}$$

with $g_1^{(j+1)}(n) = o(g_1^{(j)}(n))$, $\rho_n = o(g_1^{(k)}(n))$ for $n \rightarrow \infty$. Let us consider an operator L of the form (193) for which we know a basis of solutions $\{\{u_n^{(j)}\}\}$, $j = 1, \dots, k$, and each one can be written as

$$u_n^{(j)} \sim \sum_{m=1}^{\infty} \alpha_m^{(j)} g_m^{(j)}(n), \quad g_{m+1}^{(j)}(n) = o(g_m^{(j)}(n)) \tag{283}$$

as $n \rightarrow \infty$ for all $m \in \mathbb{N}$ and $j = 1, \dots, k$. Suppose that

- (a) $g_2^{(j+1)}(n) = o(g_2^{(j)}(n))$ for $n \rightarrow \infty$, $j = 1, \dots, k - 1$,
 - (b) $g_2^{(1)}(n) = o(g_1^{(k)}(n))$, and $\rho_n \sim Kg_2^{(1)}(n)$ for $n \rightarrow \infty$,
 - (c) $\{\{g_m^{(j)}(n)\}\}$ has property M for $m \in \mathbb{N}$, $j = 1, \dots, k$.
- (284)

Then

1. *If $\{\{\omega_n\}\}$ satisfies $\lim_{n \rightarrow \infty} \omega_n/\omega_{n+1} = \lambda \neq 1$, the sequence transformation $\mathcal{F}_n^{(k+1)}$ corresponding to the operator L accelerates the convergence of $\{\{s_n\}\}$. Moreover, the acceleration can be measured by*

$$\frac{\mathcal{F}_n^{(k+1)} - s}{s_n - s} \sim Cn^{-k} \frac{g_2^{(1)}(n)}{g_1^{(1)}(n)}, \quad n \rightarrow \infty. \tag{285}$$

2. *If $\{\{1/\omega_n\}\}$ has property M , then the speed of convergence of $\mathcal{F}_n^{(k+1)}$ can be measured by*

$$\frac{\mathcal{F}_n^{(k+1)} - s}{s_n - s} \sim C \frac{g_2^{(1)}(n)}{g_1^{(1)}(n)}, \quad n \rightarrow \infty. \tag{286}$$

7.2. Results for special cases

In the case that peculiar properties of a Levin-type sequence transformation are used, more stringent theorems can often be proved as regards convergence acceleration using this particular transformation.

In the case of the Levin transformation, Sidi proved the following theorem:

Theorem 15 (Sidi [76] and Brezowski and Redivo Zaglia [14, Theorem 2.32]). *If $s_n = s + \omega_n f_n$ where $f_n \sim \sum_{j=0}^{\infty} \beta_j/n^j$ with $\beta_0 \neq 0$ and $\omega_n \sim \sum_{j=0}^{\infty} \delta_j/n^{j+a}$ with $a > 0$, $\delta_0 \neq 0$ for $n \rightarrow \infty$ then, if $\beta_k \neq 0$*

$$\mathcal{L}_n^{(k)} - s \sim \frac{\delta_0 \beta_k}{\binom{-a}{k}} \cdot n^{-a-k} \quad (n \rightarrow \infty). \tag{287}$$

For the W algorithm and the $d^{(1)}$ transformation that may be regarded as direct generalizations of the Levin transformation, Sidi has obtained a large number of results. The interested reader is referred to the literature (see [77,78] and references therein).

Convergence results for the Levin transformation, the Drummond transformation and the Weniger transformations may be found in Section 13 of Weniger’s report [84].

Results for the \mathcal{J} transformation and in particular, for the ${}_p\mathbf{J}$ transformation are given in [39,40]. Here, we recall the following theorems:

Theorem 16. *Assume that the following holds:*

- (A-0) *The sequence $\{\{s_n\}\}$ has the (anti)limit s .*
- (A-1a) *For every n , the elements of the sequence $\{\{\omega_n\}\}$ are strictly alternating in sign and do not vanish.*
- (A-1b) *For all n and k , the elements of the sequence $\{\{\delta_n^{(k)}\}\} = \{\{\Delta r_n^{(k)}\}\}$ are of the same sign and do not vanish.*
- (A-2) *For all $n \in \mathbb{N}_0$ the ratio $(s_n - s)/\omega_n$ can be expressed as a series of the form*

$$\frac{s_n - s}{\omega_n} = c_0 + \sum_{j=1}^{\infty} c_j \sum_{n > n_1 > n_2 > \dots > n_j} \delta_{n_1}^{(0)} \delta_{n_2}^{(1)} \dots \delta_{n_j}^{(j-1)} \tag{288}$$

with $c_0 \neq 0$.

Then the following holds for $s_n^{(k)} = \mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{\delta_n^{(k)}\}\})$:

- (a) *The error $s_n^{(k)} - s$ satisfies*

$$s_n^{(k)} - s = \frac{b_n^{(k)}}{\nabla_n^{(k-1)} \nabla_n^{(k-2)} \dots \nabla_n^{(0)} [1/\omega_n]} \tag{289}$$

with

$$b_n^{(k)} = c_k + \sum_{j=k+1}^{\infty} c_j \sum_{n > n_{k+1} > n_{k+2} > \dots > n_j} \delta_{n_{k+1}}^{(k)} \delta_{n_{k+2}}^{(k+1)} \dots \delta_{n_j}^{(j-1)}. \tag{290}$$

- (b) *The error $s_n^{(k)} - s$ is bounded in magnitude according to*

$$|s_n^{(k)} - s| \leq |\omega_n b_n^{(k)} \delta_n^{(0)} \delta_n^{(1)} \dots \delta_n^{(k-1)}|. \tag{291}$$

- (c) *For large n the estimate*

$$\frac{s_n^{(k)} - s}{s_n - s} = O(\delta_n^{(0)} \delta_n^{(1)} \dots \delta_n^{(k-1)}) \tag{292}$$

holds if $b_n^{(k)} = O(1)$ and $(s_n - s)/\omega_n = O(1)$ as $n \rightarrow \infty$.

Theorem 17. *Define $s_n^{(k)} = \mathcal{J}_n^{(k)}(\{\{s_n\}\}, \{\{\omega_n\}\}, \{\{\delta_n^{(k)}\}\})$ and $\omega_n^{(k)} = 1/D_n^{(k)}$ where the $D_n^{(k)}$ are defined as in Eq. (94). Put $e_n^{(k)} = 1 - \omega_{n+1}^{(k)}/\omega_n^{(k)}$ and $b_n^{(k)} = (s_n^{(k)} - s)/\omega_n^{(k)}$. Assume that (A-0) of Theorem 16 holds and that the following conditions are satisfied:*

- (B-1) *Assume that*

$$\lim_{n \rightarrow \infty} \frac{b_n^{(k)}}{b_n^{(0)}} = B_k \tag{293}$$

exists and is finite.

- (B-2) *Assume that*

$$\Omega_k = \lim_{n \rightarrow \infty} \frac{\omega_{n+1}^{(k)}}{\omega_n^{(k)}} \neq 0 \tag{294}$$

and

$$F_k = \lim_{n \rightarrow \infty} \frac{\delta_{n+1}^{(k)}}{\delta_n^{(k)}} \neq 0 \tag{295}$$

exist for all $k \in \mathbb{N}_0$. Hence the limits $\Phi_k = \lim_{n \rightarrow \infty} \Phi_n^{(k)}$ (cf. Eq. (97)) exist for all $k \in \mathbb{N}_0$. Then, the following holds:

(a) If $\Omega_0 \notin \{\Phi_0 = 1, \Phi_1, \dots, \Phi_{k-1}\}$, then

$$\lim_{n \rightarrow \infty} \frac{s_n^{(k)} - s}{s_n - s} \left\{ \prod_{l=0}^{k-1} \delta_n^{(l)} \right\}^{-1} = B_k \frac{[\Omega_0]^k}{\prod_{l=0}^{k-1} (\Phi_l - \Omega_0)} \tag{296}$$

and, hence,

$$\frac{s_n^{(k)} - s}{s_n - s} = O(\delta_n^{(0)} \delta_n^{(1)} \dots \delta_n^{(k-1)}) \tag{297}$$

holds in the limit $n \rightarrow \infty$.

(b) If $\Omega_l = 1$ for $l \in \{0, 1, 2, \dots, k\}$ then

$$\lim_{n \rightarrow \infty} \frac{s_n^{(k)} - s}{s_n - s} \left\{ \prod_{l=0}^{k-1} \frac{\delta_n^{(l)}}{e_n^{(l)}} \right\}^{-1} = B_k \tag{298}$$

and, hence,

$$\frac{s_n^{(k)} - s}{s_n - s} = O\left(\prod_{l=0}^{k-1} \frac{\delta_n^{(l)}}{e_n^{(l)}}\right) \tag{299}$$

holds in the limit $n \rightarrow \infty$.

This theorem has the following two corollaries for the ${}_p\mathbf{J}$ transformation [39]:

Corollary 18. Assume that the following holds:

(C-1) Let $\beta > 0$, $p \geq 1$ and $\delta_n^{(k)} = \Delta[(n + \beta + (p - 1)k)^{-1}]$. Thus, we deal with the ${}_p\mathbf{J}$ transformation and, hence, the equations $F_k = \lim_{n \rightarrow \infty} \delta_{n+1}^{(k)} / \delta_n^{(k)} = 1$ and $\Phi_k = 1$ hold for all k .

(C-2) Assumptions (A-2) of Theorem 16 and (B-1) of Theorem 17 are satisfied for the particular choice (C-1) for $\delta_n^{(k)}$.

(C-3) The limit $\Omega_0 = \lim_{n \rightarrow \infty} \omega_{n+1} / \omega_n$ exists, and it satisfies $\Omega_0 \notin \{0, 1\}$. Hence, all the limits $\Omega_k = \lim_{n \rightarrow \infty} \omega_{n+1}^{(k)} / \omega_n^{(k)}$ exist for $k \in \mathbb{N}$ exist and satisfy $\Omega_k = \Omega_0$.

Then the transformation $s_n^{(k)} = {}_p\mathbf{J}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\})$ satisfies

$$\lim_{n \rightarrow \infty} \frac{s_n^{(k)} - s}{s_n - s} \left\{ \prod_{l=0}^{k-1} \delta_n^{(l)} \right\}^{-1} = B_k \left\{ \frac{\Omega_0}{1 - \Omega_0} \right\}^k \tag{300}$$

and, hence,

$$\frac{s_n^{(k)} - s}{s_n - s} = O((n + \beta)^{-2k}) \tag{301}$$

holds in the limit $n \rightarrow \infty$.

Note that Corollary 18 can be applied in the case of linear convergence because then $0 < |\Omega_0| < 1$ holds.

Corollary 18 allows to conclude that in the case of linear convergence, the ${}_p\mathbf{J}$ transformations should be superior to Wynn’s epsilon algorithm [104]. Consider for instance the case that

$$s_n \sim s + \lambda^n n^\theta \sum_{n=0}^{\infty} c_j/n^j, \quad c_0 \neq 0, \quad n \rightarrow \infty \tag{302}$$

is an asymptotic expansion of the sequence elements s_n . Assuming $\lambda \neq 1$ and $\theta \notin \{0, 1, \dots, k - 1\}$ it follows that [102, p. 127; 84, p. 333, Eq. (13.4–7)]

$$\frac{\varepsilon_{2k}^{(n)} - s}{s_n - s} = O(n^{-2k}), \quad n \rightarrow \infty. \tag{303}$$

This is the same order of convergence acceleration as in Eq. (301). But it should be noted that for the computation of $\varepsilon_{2k}^{(n)}$ the $2k + 1$ sequence elements $\{s_n, \dots, s_{n+2k}\}$ are required. But for the computation of ${}_p\mathbf{J}_n^{(k)}$ only the $k + 1$ sequence elements $\{s_n, \dots, s_{n+k}\}$ are required in the case of the t and u variants, and additionally s_{n+k+1} in the case of the \tilde{t} variant. Again, this is similar to Levin-type accelerators [84, p. 333].

The following corollary applies to the case of logarithmic convergence:

Corollary 19. *Assume that the following holds:*

- (D-1) *Let $\beta > 0, p \geq 1$ and $\delta_n^{(k)} = \Delta[(n + \beta + (p - 1)k)^{-1}]$. Thus, we deal with the ${}_p\mathbf{J}$ transformation and, hence, the equations $F_k = \lim_{n \rightarrow \infty} \delta_{n+1}^{(k)}/\delta_n^{(k)} = 1$ and $\Phi_k = 1$ hold for all k .*
- (D-2) *Assumptions (A-2) of Theorem 16 and (B-1) of Theorem 15 are satisfied for the particular choice (C-1) for $\delta_n^{(k)}$.*
- (D-3) *Some constants $a_l^{(j)}, j = 1, 2$, exist such that*

$$e_n^{(l)} = 1 - \omega_{n+1}^{(l)}/\omega_n^{(l)} = \frac{a_l^{(1)}}{n + \beta} + \frac{a_l^{(2)}}{(n + \beta)^2} + O((n + \beta)^{-3}) \tag{304}$$

holds for $l=0$. This implies that this equation, and hence, $\Omega_l=1$ holds for $l \in \{0, 1, 2, \dots, k\}$.

Assume further that $a_l^{(1)} \neq 0$ for $l \in \{0, 1, 2, \dots, k - 1\}$.

Then the transformation $s_n^{(k)} = {}_p\mathbf{J}_n^{(k)}(\beta, \{\{s_n\}\}, \{\{\omega_n\}\})$ satisfies

$$\lim_{n \rightarrow \infty} \frac{s_n^{(k)} - s}{s_n - s} \left\{ \prod_{l=0}^{k-1} \frac{\delta_n^{(l)}}{e_n^{(l)}} \right\}^{-1} = B_k \tag{305}$$

and, hence,

$$\frac{s_n^{(k)} - s}{s_n - s} = O((n + \beta)^{-k}) \tag{306}$$

holds in the limit $n \rightarrow \infty$.

For convergence acceleration results regarding the \mathcal{H} and \mathcal{S} transformations, see [34,44].

8. Stability results for Levin-type transformations

8.1. General results

We remind the reader of the definition of the *stability indices* $\Gamma_n^{(k)}(\mathcal{T}) \geq 1$ as given in Eq. (76). We consider the sequence $\{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}}$ as given. We call the transformation \mathcal{T} *stable along the path* $\mathcal{P} = \{(n_\ell, k_\ell) \mid [n_\ell > n_{\ell-1} \text{ and } k_\ell \geq k_{\ell-1}] \text{ or } [n_\ell \geq n_{\ell-1} \text{ and } k_\ell > k_{\ell-1}]\}$ in the \mathcal{T} table if the limit of its stability index along the path \mathcal{P} exists and is bounded, i.e., if

$$\lim_{\ell \rightarrow \infty} \Gamma_{n_\ell}^{(k_\ell)}(\mathcal{T}) = \lim_{\ell \rightarrow \infty} \sum_{j=0}^{k_\ell} |\gamma_{n_\ell, j}(k_\ell)(\omega_n)| < \infty, \tag{307}$$

where the $\gamma_{n, j}^{(k)}(\omega_n)$ are defined in Eq. (75). The transformation \mathcal{T} is called *S-stable*, if it is stable along all paths $\mathcal{P}^{(k)} = \{(n, k) \mid n = 0, 1, \dots\}$ for fixed k , i.e., along all columns in the \mathcal{T} table.

The case of stability along diagonal paths is much more difficult to treat analytically unless Theorem 22 applies. Up to now it seems that such diagonal stability issues have only been analysed by Sidi for the case of the $d^{(1)}$ transformation (see [78] and references therein). We will treat only S-stability in the sequel.

The higher the stability index $\Gamma(\mathcal{T})$ is, the smaller is the numerical stability of the transformation \mathcal{T} : If ε_j is the numerical error of s_j ,

$$\varepsilon_j = s_j - \text{fl}(s_j), \tag{308}$$

then the difference between the true value $\mathcal{T}_n^{(k)}$ and the numerically computed approximation $\text{fl}(\mathcal{T}_n^{(k)})$ may be bounded according to

$$|\mathcal{T}_n^{(k)} - \text{fl}(\mathcal{T}_n^{(k)})| \leq \Gamma_n^{(k)}(\mathcal{T}) \left(\max_{j \in \{0, 1, \dots, k\}} |\varepsilon_{n+j}| \right), \tag{309}$$

cf. also [78].

Theorem 20. *If the Levin-type sequence transformation $\mathcal{T}^{(k)}$ has a limiting transformation $\overset{\circ}{\mathcal{T}}^{(k)}$ with characteristic polynomial $\overset{\circ}{\Pi}^{(k)} \in \mathbb{P}^{(k)}$ for all $k \in \mathbb{N}$, and if $\{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}}$ satisfies $\omega_{n+1}/\omega_n \sim \rho \neq 0$ for large n with $\overset{\circ}{\Pi}^{(k)}(1/\rho) \neq 0$ for all $k \in \mathbb{N}$ then the transformation \mathcal{T} is S-stable. If additionally, the coefficients $\overset{\circ}{\lambda}_j^{(k)}$ of the characteristic polynomial alternate in sign, i.e., if $\overset{\circ}{\lambda}_j^{(k)} = (-1)^j |\overset{\circ}{\lambda}_j^{(k)}|/\tau_k$ with $|\tau_k| = 1$, then the limits $\overset{\circ}{\Gamma}^{(k)}(\mathcal{T}) = \lim_{n \rightarrow \infty} \Gamma_n^{(k)}(\mathcal{T})$ obey*

$$\overset{\circ}{\Gamma}^{(k)}(\mathcal{T}) = \tau_k \frac{\overset{\circ}{\Pi}^{(k)}(-1/|\rho|)}{|\overset{\circ}{\Pi}^{(k)}(1/\rho)|}. \tag{310}$$

Proof. We have for fixed k

$$\gamma_{n, j}^{(k)}(\omega_n) = \lambda_{n, j}^{(k)} \frac{\omega_n}{\omega_{n+j}} \left[\sum_{j'=0}^k \lambda_{n, j'}^{(k)} \frac{\omega_n}{\omega_{n+j'}} \right]^{-1} \sim \overset{\circ}{\lambda}_j^{(k)} \rho^{-j} \left[\sum_{j'=0}^k \overset{\circ}{\lambda}_{j'}^{(k)} \rho^{-j'} \right]^{-1} = \frac{\overset{\circ}{\lambda}_j^{(k)} \rho^{-j}}{\overset{\circ}{\Pi}^{(k)}(1/\rho)}, \tag{311}$$

whence

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)}(\mathcal{T}) = \lim_{n \rightarrow \infty} \sum_{j=0}^k |\gamma_{n,j}^{(k)}(\omega_n)| = \frac{\sum_{j=0}^k |\overset{\circ}{\lambda}_j^{(k)}| |\rho|^{-j}}{|\overset{\circ}{\Pi}^{(k)}(1/\rho)|} < \infty. \tag{312}$$

If the $\overset{\circ}{\lambda}_j^{(k)}$ alternate in sign, we obtain for these limits

$$\overset{\circ}{\Gamma}^{(k)}(\mathcal{T}) = \tau_k \frac{\sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} (-|\rho|)^{-j}}{|\overset{\circ}{\Pi}^{(k)}(1/\rho)|}. \tag{313}$$

This implies Eq. (310). \square

Corollary 21. *Assume that the Levin-type sequence transformation $\mathcal{T}^{(k)}$ has a limiting transformation $\overset{\circ}{\mathcal{T}}^{(k)}$ with characteristic polynomial $\overset{\circ}{\Pi}^{(k)} \in \mathbb{P}^{(k)}$ and the coefficients $\overset{\circ}{\lambda}_j^{(k)}$ of the characteristic polynomial alternate in sign, i.e., if $\overset{\circ}{\lambda}_j^{(k)} = (-1)^j |\overset{\circ}{\lambda}_j^{(k)}| / \tau_k$ with $|\tau_k| = 1$ for all $k \in \mathbb{N}$. The sequence $\{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}}$ is assumed to be alternating and to satisfy $\omega_{n+1}/\omega_n \sim \rho < 0$ for large n . Then the transformation \mathcal{T} is S -stable. Additionally the limits are $\overset{\circ}{\Gamma}^{(k)}(\mathcal{T}) = 1$.*

Proof. Since

$$\begin{aligned} \sum_{j'=0}^k \frac{\lambda_{n,j'}^{(k)}}{\tau_k^{-1}} \frac{\omega_n}{\omega_{n+j'}} &\sim \frac{\overset{\circ}{\Pi}^{(k)}(1/\rho)}{\tau_k^{-1}} = \sum_{j'=0}^k \frac{\overset{\circ}{\lambda}_{j'}^{(k)}}{\tau_k^{-1}} (-1)^{j'} |\rho|^{-j'} \\ &= \sum_{j'=0}^k |\overset{\circ}{\lambda}_{j'}^{(k)}| |\rho|^{-j'} \geq |\overset{\circ}{\lambda}_k^{(k)}| / |\rho|^k > 0. \end{aligned} \tag{314}$$

$1/\rho$ cannot be a zero of $\overset{\circ}{\Pi}^{(k)}$. Then, Theorem 20 entails that \mathcal{T} is S -stable. Furthermore, Eq. (310) is applicable and yields $\overset{\circ}{\Gamma}^{(k)}(\mathcal{T}) = 1$. \square

This result can be improved if all the coefficients $\lambda_{n,j}^{(k)}$ are alternating:

Theorem 22. *Assume that the Levin-type sequence transformation $\mathcal{T}^{(k)}$ has a characteristic polynomials $\Pi_n^{(k)} \in \mathbb{P}^{(k)}$ with alternating coefficients $\lambda_{n,j}^{(k)}$ i.e., $\lambda_{n,j}^{(k)} = (-1)^j |\lambda_{n,j}^{(k)}| / \tau_k$ with $|\tau_k| = 1$ for all $n \in \mathbb{N}_0$ and $k \in \mathbb{N}$. The sequence $\{\{\omega_n\}\} \in \mathbb{O}^{\mathbb{K}}$ is assumed to be alternating and to satisfy $\omega_{n+1}/\omega_n < 0$ for all $n \in \mathbb{N}_0$. Then we have $\Gamma_n^{(k)}(\mathcal{T}) = 1$. Hence, the transformation \mathcal{T} is stable along all paths for such remainder estimates.*

Proof. We have for fixed n and k

$$\gamma_{n,j}^{(k)}(\omega_n) = \frac{\lambda_{n,j}^{(k)} \omega_n / \omega_{n+j}}{\sum_{j'=0}^k \lambda_{n,j'}^{(k)} \omega_n / \omega_{n+j'}} = \frac{\lambda_{n,j}^{(k)} \tau_k (-1)^j |\omega_n / \omega_{n+j}|}{\sum_{j'=0}^k \lambda_{n,j'}^{(k)} \tau_k (-1)^{j'} |\omega_n / \omega_{n+j'}|} = \frac{|\lambda_{n,j}^{(k)}| |\omega_n / \omega_{n+j}|}{\sum_{j'=0}^k |\lambda_{n,j'}^{(k)}| |\omega_n / \omega_{n+j'}|} \geq 0. \tag{315}$$

Note that the denominators cannot vanish and are bounded from below by $|\lambda_{n,k}^{(k)}\omega_n/\omega_{n+k}| > 0$. Hence, we have $\gamma_{n,j}^{(k)}(\omega_n) = |\gamma_{n,j}^{(k)}(\omega_n)|$ and consequently, $\Gamma_n^{(k)}(\mathcal{T}) = 1$ since $\sum_{j=0}^k \gamma_{n,j}^{(k)}(\omega_n) = 1$ according to Eq. (75). \square

8.2. Results for special cases

Here, we collect some special results on the stability of various Levin-type sequence transformations that have been reported in [46] and generalize some results of Sidi on the S -stability of the $d^{(1)}$ transformation.

Theorem 23. *If the sequence ω_{n+1}/ω_n possesses a limit according to*

$$\lim_{n \rightarrow \infty} \omega_{n+1}/\omega_n = \rho \neq 0 \tag{316}$$

and if $\rho \notin \{1, \Phi_1, \dots, \Phi_k, \dots\}$ such that the limiting transformation exists, the \mathcal{J} transformation is S -stable with the same limiting stability indices as the transformation $\overset{\circ}{\mathcal{J}}$, i.e., we have

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)} = \frac{\sum_{j=0}^k |\lambda_j^{(k)} \rho^{k-j}|}{\prod_{j'=0}^{k-1} |\Phi_{j'} - \rho|} < \infty. \tag{317}$$

If all Φ_k are positive then

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)} = \prod_{j=0}^{k-1} \frac{\Phi_j + |\rho|}{|\Phi_j - \rho|} < \infty \tag{318}$$

holds.

As corollaries, we get the following results

Corollary 24. *If the sequence ω_{n+1}/ω_n possesses a limit according to*

$$\lim_{n \rightarrow \infty} \omega_{n+1}/\omega_n = \rho \notin \{0, 1\}, \tag{319}$$

the ${}_p\mathbf{J}$ transformation for $p > 1$ and $\beta > 0$ is S -stable and we have

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)} = \frac{\sum_{j=0}^k \binom{k}{j} |\rho^{k-j}|}{|1 - \rho|^k} = \frac{(1 + |\rho|)^k}{|1 - \rho|^k} < \infty. \tag{320}$$

Corollary 25. *If the sequence ω_{n+1}/ω_n possesses a limit according to*

$$\lim_{n \rightarrow \infty} \omega_{n+1}/\omega_n = \rho \notin \{0, 1\}, \tag{321}$$

the Weniger \mathcal{S} transformation [84, Section 8] for $\beta > 0$ is S -stable and we have

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)}(\mathcal{S}) = \frac{\sum_{j=0}^k \binom{k}{j} |\rho^{k-j}|}{|1 - \rho|^k} = \frac{(1 + |\rho|)^k}{|1 - \rho|^k} < \infty. \tag{322}$$

Corollary 26. *If the sequence ω_{n+1}/ω_n possesses a limit according to*

$$\lim_{n \rightarrow \infty} \omega_{n+1}/\omega_n = \rho \notin \{0, 1\}, \tag{323}$$

the Levin \mathcal{L} transformation [53, 84] is S -stable and we have

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)}(\mathcal{L}) = \frac{\sum_{j=0}^k \binom{k}{j} |\rho^{k-j}|}{|1 - \rho|^k} = \frac{(1 + |\rho|)^k}{|1 - \rho|^k} < \infty. \tag{324}$$

Corollary 27. *Assume that the elements of the sequence $\{t_n\}_{n \in \mathbb{N}}$ satisfy $t_n \neq 0$ for all n and $t_n \neq t_{n'}$ for all $n \neq n'$. If the sequence t_{n+1}/t_n possesses a limit*

$$\lim_{n \rightarrow \infty} t_{n+1}/t_n = \tau \quad \text{with } 0 < \tau < 1 \tag{325}$$

and if the sequence ω_{n+1}/ω_n possesses a limit according to

$$\lim_{n \rightarrow \infty} \omega_{n+1}/\omega_n = \rho \notin \{0, 1, \tau^{-1}, \dots, \tau^{-k}, \dots\}, \tag{326}$$

then the generalized Richardson extrapolation process \mathcal{R} introduced by Sidi [73] that is identical to the \mathcal{J} transformation with $\delta_n^{(k)} = t_n - t_{n+k+1}$ as shown in [36], i.e., the W algorithm is S -stable and we have

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)}(\mathcal{R}) = \frac{\sum_{j=0}^k |\tilde{\lambda}_j^{(k)} \rho^{k-j}|}{\prod_{j'=0}^{k-1} |\tau^{-j'} - \rho|} = \prod_{j'=0}^{k-1} \frac{1 + \tau^{j'} |\rho|}{|1 - \tau^{j'} \rho|} < \infty. \tag{327}$$

Here

$$\tilde{\lambda}_j^{(k)} = (-1)^{k-j} \sum_{\substack{j_0 + j_1 + \dots + j_{k-1} = j, \\ j_0 \in \{0, 1\}, \dots, j_{k-1} \in \{0, 1\}}} \prod_{m=0}^{k-1} (\tau)^{-m j_m}, \tag{328}$$

such that

$$\sum_{j=0}^k \tilde{\lambda}_j^{(k)} \rho^{k-j} = \prod_{j=0}^{k-1} (\tau^{-j} - \rho) = \tau^{-k(k-1)/2} \prod_{j=0}^{k-1} (1 - \tau^j \rho). \tag{329}$$

Note that the preceding corollary is essentially the same as a result of Sidi [78, Theorem 2.2] that now appears as a special case of the more general Theorem 23 that applies to a much wider class of sequence transformations. As noted above, Sidi has also derived conditions under which the $d^{(1)}$ transformation is stable along the paths $\mathcal{P}_n = \{(n, k) | k = 0, 1, \dots\}$ for fixed n . For details and more references see [78]. Analogous work for the \mathcal{J} transformation is in progress.

An efficient algorithm for the computation of the stability index of the \mathcal{J} transformation can be given in the case $\delta_n^{(k)} > 0$. Since the \mathcal{J} transformation is invariant under $\delta_n^{(k)} \rightarrow \alpha^{(k)} \delta_n^{(k)}$ for any $\alpha^{(k)} \neq 0$ according to Homeier [36, Theorem 4], $\delta_n^{(k)} > 0$ can always be achieved if for given k , all $\delta_n^{(k)}$ have the same sign. This is the case, for instance, for the ${}_p\mathbf{J}$ transformation [36,39].

Theorem 28. Define

$$F_n^{(0)} = (-1)^n |D_n^{(0)}|, \quad F_n^{(k+1)} = (F_{n+1}^{(k)} - F_n^{(k)}) / \delta_n^{(k)} \tag{330}$$

and $\hat{F}_n^{(0)} = F_n^{(0)}$, $\hat{F}_n^{(k)} = (\delta_n^{(0)} \dots \delta_n^{(k-1)}) F_n^{(k)}$. If all $\delta_n^{(k)} > 0$ then

1. $F_n^{(k)} = (-1)^{n+k} |F_n^{(k)}|$,
2. $\lambda_{n,j}^{(k)} = (-1)^{j+k} |\lambda_{n,j}^{(k)}|$, and
- 3.

$$\Gamma_n^{(k)} = \frac{|\hat{F}_n^{(k)}|}{|\hat{D}_n^{(k)}|} = \frac{|F_n^{(k)}|}{|D_n^{(k)}|}. \tag{331}$$

This generalizes Sidi’s method for the computation of stability indices [78] to a larger class of sequence transformations.

9. Application of Levin-type sequence transformations

9.1. Practical guidelines

Here, we address shortly the following questions:

When should one try to use sequence transformations? One can only hope for good convergence acceleration, extrapolation, or summation results if (a) the s_n have some asymptotic structure for large n and are not erratic or random, (b) a sufficiently large number of decimal digits is available. Many problems can be successfully tackled if 13–15 digits are available but some require a much larger number of digits in order to overcome some inevitable rounding errors, especially for the acceleration of logarithmically convergent sequences. The asymptotic information that is required for a successful extrapolation is often hidden in the last digits of the problem data.

How should the transformations be applied? The recommended mode of application is that one computes the highest possible order k of the transformation from the data. In the case of triangular recursive schemes like that of the \mathcal{J} transformation and the Levin transformation, this means that one computes as transformed sequence $\{\mathcal{T}_0^{(n)}\}$. For L-shaped recursive schemes as in the case of the \mathcal{H} , \mathcal{I} , and \mathcal{K} transformations, one usually computes as transformed sequence $\{\{\mathcal{T}_{n-2\lfloor n/2 \rfloor}^{\lfloor n/2 \rfloor}\}\}$. The error ε of the current estimate can usually be approximated a posteriori using sums of magnitudes of differences of a few entries of the \mathcal{T} table, e.g.,

$$\varepsilon \approx |\mathcal{T}_1^{(n)} - \mathcal{T}_0^{(n)}| + |\mathcal{T}_0^{(n-1)} - \mathcal{T}_0^{(n)}| \tag{332}$$

for transformations with triangular recursive schemes. Such a simple approach works surprisingly well in practice. The loss of decimal digits can be estimated computing stability indices. An example is given below.

What happens if one of the denominator vanishes? The occurrence of zeroes in the D table for specific combinations of n and k is usually no problem since the recurrences for numerators and denominators still work in this case. Thus, no special devices are required to jump over such singular points in the \mathcal{T} table.

Which transformation and which variant should be chosen? This depends on the type of convergence of the problem sequence. For linearly convergent sequences, t , \tilde{t} , u and v variants of the Levin transformation, or the ${}_p\mathbf{J}$ transformation, especially the ${}_2\mathbf{J}$ transformation are usually a good choice [39] as long as one is not too close to a singularity or to a logarithmically convergent problem. Especially well behaved is usually the application to alternating series since then, the stability is very good as discussed above. For the summation of alternating divergent sequences and series, usually the t and the \tilde{t} variants of the Levin transformation, the ${}_2\mathbf{J}$ and the Weniger \mathcal{S} and \mathcal{M} transformations provide often surprisingly accurate results. In the case of logarithmic convergence, t and \tilde{t} variants become useless, and the order of acceleration is dropping from $2k$ to k when the transformation is used columnwise. If a Kummer-related series is available (cf. Section 2.2.1), then K and lu variants leading to linear sequence transformations can be efficient [50]. Similarly, linear variants can be based on some good asymptotic estimates ${}^{\text{asy}}\omega_n$, that have to be obtained via a separate analysis [50]. In the case of logarithmic convergence, it pays to consider special devices like using subsequences $\{\{s_{\xi_n}\}\}$ where the ξ_n grow exponentially like $\xi_n = \lfloor \sigma \xi_{n-1} \rfloor + 1$ like in the d transformations. This choice can be also used in combination with the \mathcal{F} transformation. Alternatively, one can use some other transformations like the condensation transformation [51,65] or interpolation to generate a linearly convergent sequence [48], before applying an usually nonlinear sequence transformation. A somewhat different approach is possible if one can obtain a few terms a_n with large n easily [47].

What to do near a singularity? When extrapolating power series or, more generally, sequences depending on certain parameters, quite often extrapolation becomes difficult near the singularities of the limit function. In the case of linear convergence, one can often transform to a problem with a larger distance to the singularity: If Eq. (28) holds, then the subsequence $\{\{s_{\tau_n}\}\}$ satisfies

$$\lim_{n \rightarrow \infty} (s_{\tau(n+1)} - s) / (s_{\tau n} - s) = \rho^\tau. \tag{333}$$

This is a method of Sidi that has can, however, be applied to large classes of sequence transformations [46].

What to do for more complicated convergence type? Here, one should try to rewrite the problem sequence as a sum of sequences with more simple convergence behavior. Then, nonlinear sequence transformations are used to extrapolate each of these simpler series, and to sum the extrapolation results to obtain an estimate for the original problem. This is for instance often possible for (generalized) Fourier series where it leads to complex series that may asymptotically be regarded as power series. For details, the reader is referred to the literature [14,35,40–45,77]. If this approach is not possible one is forced to use more complicated sequence transformations like the $d^{(m)}$ transformations or the (generalized) \mathcal{H} transformation. These more complicated sequence transformations, however, do require more numerical effort to achieve a desired accuracy.

9.2. Numerical examples

In Table 3, we present results of the application of certain variants of the \mathcal{F} transformation and the W algorithm to the series

$$S(z, a) = 1 + \sum_{j=1}^{\infty} z^j \prod_{\ell=0}^{j-1} \frac{1}{\ln(a + \ell)} \tag{334}$$

Table 3
Comparison of the \mathcal{F} transformation and the W algorithm for series (334)^a

n	A_n	B_n	C_n	D_n
14	13.16	13.65	7.65	11.13
16	15.46	15.51	9.43	12.77
18	18.01	17.84	11.25	14.43
20	21.18	20.39	13.10	16.12
22	23.06	23.19	14.98	17.81
24	25.31	26.35	16.89	19.53
26	27.87	28.17	18.83	21.26
28	30.83	30.59	20.78	23.00
30	33.31	33.19	22.76	24.76
n	E_n	F_n	G_n	H_n
14	14.07	13.18	9.75	10.47
16	15.67	15.49	11.59	12.05
18	17.94	18.02	13.46	13.66
20	20.48	20.85	15.37	15.29
22	23.51	23.61	17.30	16.95
24	25.66	25.63	19.25	18.62
26	27.89	28.06	21.23	20.31
28	30.46	30.67	23.22	22.02
29	31.82	32.20	24.23	22.89
30	33.43	33.45	25.24	23.75

^aPlotted is the negative decadic logarithm of the relative error.

- A_n : $\mathcal{F}_0^{(n)}(\{\{S_n(z, a)\}, \{(2 + \ln(n + a)) \Delta S_n(z, a)\}, \{1 + \ln(n + a)\}\})$,
- B_n : $W_0^{(n)}(\{\{S_n(z, a)\}, \{(2 + \ln(n + a)) \Delta S_n(z, a)\}, \{1/(1 + \ln(n + a))\}\})$,
- C_n : $\mathcal{F}_0^{(n)}(\{\{S_n(z, a)\}, \{(n + 1) \Delta S_n(z, a)\}, \{1 + n + a\}\})$,
- D_n : $W_0^{(n)}(\{\{S_n(z, a)\}, \{(n + 1) \Delta S_n(z, a)\}, \{1/(1 + n + a)\}\})$,
- E_n : $\mathcal{F}_0^{(n)}(\{\{S_n(z, a)\}, \{\Delta S_n(z, a)\}, \{1 + \ln(n + a)\}\})$,
- F_n : $W_0^{(n)}(\{\{S_n(z, a)\}, \{\Delta S_n(z, a)\}, \{1/(1 + \ln(n + a))\}\})$,
- G_n : $\mathcal{F}_0^{(n)}(\{\{S_n(z, a)\}, \{\Delta S_n(z, a)\}, \{1 + n + a\}\})$,
- H_n : $W_0^{(n)}(\{\{S_n(z, a)\}, \{\Delta S_n(z, a)\}, \{1/(1 + n + a)\}\})$.

with partial sums

$$S_n(z, a) = 1 + \sum_{j=1}^n z^j \prod_{\ell=0}^{j-1} \frac{1}{\ln(a + \ell)} \tag{335}$$

for $z = 1.2$ and $a = 1.01$. Since the terms a_j satisfy $a_{j+1}/a_j = z/\ln(a + j)$, the ratio test reveals that $S(z, a)$ converges for all z and, hence, represents an analytic function. Nevertheless, only for $j \geq -a + \exp(|z|)$, the ratio of the terms becomes less than unity in absolute value. Hence, for larger z the series converges rather slowly.

It should be noted that for cases C_n and G_n , the \mathcal{F} transformation is identical to the Weniger transformation \mathcal{S} , i.e., to the $3\mathbf{J}$ transformation, and for cases C_n and H_n the W algorithm is identical to the Levin transformation. In the upper part of the table, we use u -type remainder estimates while

Table 4

Acceleration of $\zeta(-1/10 + 10i, 1, 95/100)$ with the \mathcal{J} transformation^a

n	A_n	B_n	C_n	D_n	E_n	F_n	G_n	H_n
10	2.59e-05	3.46e+01	2.11e-05	4.67e+01	1.84e-05	4.14e+01	2.63e-05	3.90e+01
20	1.72e-05	6.45e+05	2.53e-05	5.53e+07	1.38e-04	3.40e+09	1.94e-05	2.47e+06
30	2.88e-05	3.52e+10	8.70e-06	2.31e+14	8.85e-05	1.22e+17	2.02e-05	6.03e+11
40	4.68e-06	1.85e+15	8.43e-08	1.27e+20	4.06e-06	2.78e+23	1.50e-06	9.27e+16
42	2.59e-06	1.46e+16	2.61e-08	1.51e+21	2.01e-06	4.70e+24	6.64e-07	8.37e+17
44	1.33e-06	1.10e+17	7.62e-09	1.76e+22	1.73e-06	7.85e+25	2.76e-07	7.24e+18
46	6.46e-07	8.00e+17	1.80e-09	2.02e+23	1.31e-05	1.30e+27	1.09e-07	6.08e+19
48	2.97e-07	5.62e+18	1.07e-08	2.29e+24	1.52e-04	2.12e+28	4.16e-08	5.00e+20
50	1.31e-07	3.86e+19	1.51e-07	2.56e+25	1.66e-03	3.43e+29	1.54e-08	4.05e+21

^a A_n : relative error of ${}_1\mathbf{J}_0^{(n)}(1, \{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\})$, B_n : stability index of ${}_1\mathbf{J}_0^{(n)}(1, \{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\})$, C_n : relative error of ${}_2\mathbf{J}_0^{(n)}(1, \{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\})$, D_n : stability index of ${}_2\mathbf{J}_0^{(n)}(1, \{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\})$, E_n : relative error of ${}_3\mathbf{J}_0^{(n)}(1, \{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\})$, F_n : stability index of ${}_3\mathbf{J}_0^{(n)}(1, \{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\})$, G_n : relative error of $\mathcal{J}_0^{(n)}(\{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\}, \{1/(n+1) - 1/(n+k+2)\})$, H_n : Stability index of $\mathcal{J}_0^{(n)}(\{\{s_n\}\}, \{(n+1)(s_n - s_{n-1})\}, \{1/(n+1) - 1/(n+k+2)\})$.

in the lower part, we use \tilde{t} variants. It is seen that the choices $x_n = 1 + \ln(a + n)$ for the \mathcal{F} transformation and $t_n = 1/(1 + \ln(a + n))$ for the W algorithm perform for both variants nearly identical (columns A_n , B_n , E_n and F_n) and are superior to the choices $x_n = 1 + n + a$ and $t_n = 1/(1 + n + a)$, respectively, that correspond to the Weniger and the Levin transformation as noted above. For the latter two transformations, the Weniger $\tilde{t}\mathcal{L}$ transformation is slightly superior the $\tilde{t}\mathcal{J}$ transformation for this particular example (columns G_n vs. H_n) while the situation is reversed for the u -type variants displayed in columns C_n and D_n .

The next example is taken from [46], namely the “inflated Riemann ζ function”, i.e., the series

$$\zeta(\varepsilon, 1, q) = \sum_{j=0}^{\infty} \frac{q^j}{(j+1)^\varepsilon}, \quad (336)$$

that is a special case of the Lerch zeta function $\zeta(s, b, z)$ (cf. [30, p. 142, Eq. (6.9.7); 20, Section 1.11]). The partial sums are defined as

$$s_n = \sum_{j=0}^n \frac{q^j}{(j+1)^\varepsilon}. \quad (337)$$

The series converges linearly for $0 < |q| < 1$ for any complex ε . In fact, we have in this case $\rho = \lim_{n \rightarrow \infty} (s_{n+1} - s)/(s_n - s) = q$. We choose $q = 0.95$ and $\varepsilon = -0.1 + 10i$. Note that for this value of ε , there is a singularity of $\zeta(\varepsilon, 1, q)$ at $q = 1$ where the defining series diverges since $\Re(\varepsilon) < 1$.

The results of applying u variants of the ${}_p\mathbf{J}$ transformation with $p = 1, 2, 3$ and of the Levin transformation to the sequence of partial sums is displayed in Table 4. For each of these four variants of the \mathcal{J} transformation, we give the relative error and the stability index. The true value of the series (that is used to compute the errors) was computed using a more accurate method described below. It is seen that the ${}_2\mathbf{J}$ transformation achieves the best results. The attainable accuracy for this transformation is limited to about 9 decimal digits by the fact that the stability index displayed in the column D_n of Table 4 grows relatively fast. Note that for $n = 46$, the number of digits (as given by

Table 5
Acceleration of $\zeta(-1/10 + 10i, 1, 95/100)$ with the \mathcal{J} transformation ($\tau = 10$)^a

n	A_n	B_n	C_n	D_n	E_n	F_n	G_n	H_n
10	2.10e - 05	2.08e + 01	8.17e - 06	3.89e + 01	1.85e - 05	5.10e + 01	1.39e - 05	2.52e + 01
12	2.49e - 06	8.69e + 01	1.43e - 07	3.03e + 02	9.47e - 06	8.98e + 02	1.29e - 06	1.26e + 02
14	1.93e - 07	3.11e + 02	5.98e - 09	1.46e + 03	8.24e - 07	4.24e + 03	6.86e - 08	5.08e + 02
16	1.11e - 08	9.82e + 02	2.02e - 11	6.02e + 03	6.34e - 08	2.09e + 04	2.57e - 09	1.77e + 03
18	5.33e - 10	2.87e + 03	1.57e - 12	2.29e + 04	4.08e - 09	9.52e + 04	7.81e - 11	5.66e + 03
20	2.24e - 11	7.96e + 03	4.15e - 14	8.26e + 04	2.31e - 10	4.12e + 05	2.07e - 12	1.73e + 04
22	8.60e - 13	2.14e + 04	8.13e - 16	2.89e + 05	1.16e - 11	1.73e + 06	4.95e - 14	5.08e + 04
24	3.07e - 14	5.61e + 04	1.67e - 17	9.87e + 05	5.17e - 13	7.07e + 06	1.10e - 15	1.46e + 05
26	1.04e - 15	1.45e + 05	3.38e - 19	3.31e + 06	1.87e - 14	2.84e + 07	2.33e - 17	4.14e + 05
28	3.36e - 17	3.69e + 05	6.40e - 21	1.10e + 07	3.81e - 16	1.13e + 08	4.71e - 19	1.16e + 06
30	1.05e - 18	9.30e + 05	1.15e - 22	3.59e + 07	1.91e - 17	4.43e + 08	9.19e - 21	3.19e + 06

^a A_n : relative error of ${}_1\mathbf{J}_0^{(n)}(1, \{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\})$, B_n : stability index of ${}_1\mathbf{J}_0^{(n)}(1, \{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\})$, C_n : relative error of ${}_2\mathbf{J}_0^{(n)}(1, \{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\})$, D_n : stability index of ${}_2\mathbf{J}_0^{(n)}(1, \{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\})$, E_n : relative error of ${}_3\mathbf{J}_0^{(n)}(1, \{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\})$, F_n : stability index of ${}_3\mathbf{J}_0^{(n)}(1, \{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\})$, G_n : relative error of $\mathcal{J}_0^{(n)}(\{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\}, \{1/(10n + 10) - 1/(10n + 10k + 10)\})$, H_n : Stability index of $H_n: \mathcal{J}_0^{(n)}(\{\{s_{10n}\}\}, \{\{(10n + 1)(s_{10n} - s_{10n-1})\}\}, \{1/(n + 1) - 1/(n + k + 2)\})$.

the negative decadic logarithm of the relative error) and the decadic logarithm of the stability index sum up to approximately 32 which corresponds to the maximal number of decimal digits that could be achieved in the run. Since the stability index increases with n , indicating decreasing stability, it is clear that for higher values of n the accuracy will be lower.

The magnitude of the stability index is largely controlled by the value of ρ , compare Corollary 24. If one can treat a related sequence with a smaller value of ρ , the stability index will be smaller and thus, the stability of the extrapolation will be greater.

Such a related sequence is given by putting $\check{s}_\ell = s_{\xi_\ell}$ for $\ell \in \mathbb{N}_0$, where the sequence ξ_ℓ is a monotonously increasing sequence of nonnegative integers. In the case of linear convergent sequences, the choice $\xi_\ell = \tau\ell$ with $\tau \in \mathbb{N}$ can be used as in the case of the $d^{(1)}$ transformation. It is easily seen that the new sequence also converges linearly with $\rho = \lim_{n \rightarrow \infty} (\check{s}_{n+1} - s) / (\check{s}_n - s) = q^\tau$. For $\tau > 1$, both the effectiveness and the stability of the various transformations are increased as shown in Table 5 for the case $\tau = 10$. Note that this value was chosen to display basic features relevant to the stability analysis, and is not necessarily the optimal value. As in Table 4, the relative errors and the stability indices of some variants of the \mathcal{J} transformation are displayed. These are nothing but the ${}_p\mathbf{J}$ transformation for $p = 1, 2, 3$ and the Levin transformation as applied to the sequence $\{\{\check{s}_n\}\}$ with remainder estimates $\omega_n = (n\tau + \beta)(s_{n\tau} - s_{n\tau-1})$ for $\beta = 1$. Since constant factors in the remainder estimates are irrelevant since the \mathcal{J} transformation is invariant under any scaling $\omega_n \rightarrow \alpha\omega_n$ for $\alpha \neq 0$, the same results would have been obtained for $\omega_n = (n + \beta/\tau)(s_{n\tau} - s_{n\tau-1})$.

If the Levin transformation is applied to the series with partial sums $\check{s}_n = s_{\tau n}$, and if the remainder estimates $\omega_n = (n + \beta/\tau)(s_{\tau n} - s_{(\tau n)-1})$ are used, then one obtains nothing but the $d^{(1)}$ transformation with $\xi_\ell = \tau\ell$ for $\tau \in \mathbb{N}$ [46,77].

Table 6
Stability indices for the ${}_2\mathbf{J}$ transformation ($\tau = 10$)

n	$\Gamma_n^{(1)}$	$\Gamma_n^{(2)}$	$\Gamma_n^{(3)}$	$\Gamma_n^{(4)}$	$\Gamma_n^{(5)}$	$\Gamma_n^{(6)}$	$\Gamma_n^{(7)}$
20	3.07	9.26	$2.70 \cdot 10^1$	$7.55 \cdot 10^1$	$2.02 \cdot 10^2$	$5.20 \cdot 10^2$	$1.29 \cdot 10^3$
30	3.54	$1.19 \cdot 10^1$	$3.81 \cdot 10^1$	$1.16 \cdot 10^2$	$3.36 \cdot 10^2$	$9.36 \cdot 10^2$	$2.51 \cdot 10^3$
40	3.75	$1.33 \cdot 10^1$	$4.49 \cdot 10^1$	$1.44 \cdot 10^2$	$4.42 \cdot 10^2$	$1.30 \cdot 10^3$	$3.71 \cdot 10^3$
41	3.77	$1.34 \cdot 10^1$	$4.54 \cdot 10^1$	$1.46 \cdot 10^2$	$4.51 \cdot 10^2$	$1.34 \cdot 10^3$	$3.82 \cdot 10^3$
42	3.78	$1.35 \cdot 10^1$	$4.59 \cdot 10^1$	$1.49 \cdot 10^2$	$4.60 \cdot 10^2$	$1.37 \cdot 10^3$	$3.93 \cdot 10^3$
43	3.79	$1.36 \cdot 10^1$	$4.64 \cdot 10^1$	$1.51 \cdot 10^2$	$4.69 \cdot 10^2$	$1.40 \cdot 10^3$	$4.05 \cdot 10^3$
44	3.80	$1.37 \cdot 10^1$	$4.68 \cdot 10^1$	$1.53 \cdot 10^2$	$4.77 \cdot 10^2$	$1.43 \cdot 10^3$	
45	3.81	$1.38 \cdot 10^1$	$4.73 \cdot 10^1$	$1.55 \cdot 10^2$	$4.85 \cdot 10^2$		
46	3.82	$1.39 \cdot 10^1$	$4.77 \cdot 10^1$	$1.57 \cdot 10^2$			
47	3.83	$1.39 \cdot 10^1$	$4.81 \cdot 10^1$				
48	3.84	$1.40 \cdot 10^1$					
49	3.85						
Extr.	4.01	$1.59 \cdot 10^1$	$6.32 \cdot 10^1$	$2.52 \cdot 10^2$	$1.00 \cdot 10^3$	$4.00 \cdot 10^3$	$1.59 \cdot 10^4$
Corollary 24	3.98	$1.59 \cdot 10^1$	$6.32 \cdot 10^1$	$2.52 \cdot 10^2$	$1.00 \cdot 10^3$	$4.00 \cdot 10^3$	$1.59 \cdot 10^4$

It is seen from Table 5 that again the best accuracy is obtained for the ${}_2\mathbf{J}$ transformation. The $d^{(1)}$ transformation is worse, but better than the ${}_p\mathbf{J}$ transformations for $p = 1$ and 3. Note that the stability indices are now much smaller and do not limit the achievable accuracy for any of the transformations up to $n=30$. The true value of the series was computed numerically by applying the ${}_2\mathbf{J}$ transformation to the further sequence $\{\{s_{40n}\}\}$ and using 64 decimal digits in the calculation. In this way, a sufficiently accurate approximation was obtained that was used to compute the relative errors in Tables 4 and 5. A comparison value was computed using the representation [20, p. 29, Eq. (8)]

$$\zeta(s, 1, q) = \frac{\Gamma(1-s)}{z} (\log 1/q)^{s-1} + z^{-1} \sum_{j=0}^{\infty} \zeta(s-j) \frac{(\log q)^j}{j!} \tag{338}$$

that holds for $|\log q| < 2\pi$ and $s \notin \mathbb{N}$. Here, $\zeta(z)$ denotes the Riemann zeta function. Both values agreed to all relevant decimal digits.

In Table 6, we display stability indices corresponding to the acceleration of \check{s}_n with the ${}_2\mathbf{J}$ transformation columnwise, as obtainable by using the sequence elements up to $\check{s}_{50} = s_{500}$. In the row labelled Corollary 24, we display the limits of the $\Gamma_n^{(k)}$ for large n , i.e., the quantities

$$\lim_{n \rightarrow \infty} \Gamma_n^{(k)} = \left(\frac{1+q^\tau}{1-q^\tau} \right)^k, \tag{339}$$

that are the limits according to Corollary 24. It is seen that the values for finite n are still relatively far off the limits. In order to check numerically the validity of the corollary, we extrapolated the values of all $\Gamma_n^{(k)}$ for fixed k with n up to the maximal n for which there is an entry in the corresponding column of Table 6 using the u variant of the ${}_1\mathbf{J}$ transformation. The results of the extrapolation are displayed in the row labelled *Extr* in Table 6 and coincide nearly perfectly with the values expected according to Corollary 24.

Table 7
 Extrapolation of series representation (340) of the $F_m(z)$ function using the ${}_2\mathbf{J}$ transformation
 ($z = 8, m = 0$)

n	s_n	${}^u\omega_n$	${}^t\omega_n$	${}^K\omega_n$
5	-13.3	0.3120747	0.3143352	0.3132981
6	-14.7	0.3132882	0.3131147	0.3133070
7	-13.1	0.3132779	0.3133356	0.3133087
8	11.4	0.3133089	0.3133054	0.3133087
9	-8.0	0.3133083	0.3133090	0.3133087

As a final example, we consider the evaluation of the $F_m(z)$ functions that are used in quantum chemistry calculations via the series representation

$$F_m(z) = \sum_{j=0}^{\infty} (-z)^j / j! (2m + 2j + 1) \tag{340}$$

with partial sums

$$s_n = \sum_{j=0}^n (-z)^j / j! (2m + 2j + 1). \tag{341}$$

In this case, for larger z , the convergence is rather slow although the convergence finally is hyper-linear. As a K variant, one may use

$${}^k\omega_n = \left(\sum_{j=0}^n (-z)^j / (j + 1)! - (1 - e^{-z}) / z \right). \tag{342}$$

since $(1 - e^{-z}) / z$ is a Kummer related series. The results for several variants in Table 7 show that the K variant is superior to u and t variants in this case.

Many further numerical examples are given in the literature [39,41–44,50,84].

Appendix A. Stieltjes series and functions

A Stieltjes series is a formal expansion

$$f(z) = \sum_{j=0}^{\infty} (-1)^j \mu_j z^j \tag{A.1}$$

with partial sums

$$f_n(z) = \sum_{j=0}^n (-1)^j \mu_j z^j. \tag{A.2}$$

The coefficients μ_n are the moments of an uniquely given positive measure $\psi(t)$ that has infinitely many different values on $0 \leq t < \infty$ [4, p. 159]:

$$\mu_n = \int_0^{\infty} t^n d\psi(t), \quad n \in \mathbb{N}_0. \tag{A.3}$$

Formally, the Stieltjes series can be identified with a Stieltjes integral

$$f(z) = \int_0^\infty \frac{d\psi(t)}{1 + zt}, \quad |\arg(z)| < \pi. \tag{A.4}$$

If such an integral exists for a function f then the function is called a Stieltjes function. For every Stieltjes function there exist a unique asymptotical Stieltjes series (A.1), uniformly in every sector $|\arg(z)| < \theta$ for all $\theta < \pi$. For any Stieltjes series, however, several different corresponding Stieltjes functions may exist. To ensure uniqueness, additional criteria are necessary [88, Section 4.3].

In the context of convergence acceleration and summation of divergent series, it is important that for given z the tails $f(z) - f_n(z)$ of a Stieltjes series are bounded in absolute value by the next term of the series,

$$|f(z) - f_n(z)| \leq \mu_{n+1} z^{n+1} \quad z \geq 0. \tag{A.5}$$

Hence, for Stieltjes series the remainder estimates may be chosen as

$$\omega_n = (-1)^{n+1} \mu_{n+1} z^{n+1}. \tag{A.6}$$

This corresponds to $\omega_n = \Delta f_n(z)$, i.e., to a \tilde{t} variant.

Appendix B. Derivation of the recursive scheme (148)

We show that for the divided difference operator $\square_n^{(k)} = \square_n^{(k)}[\{\{x_n\}\}]$ the identity

$$\square_n^{(k+1)}((x)_{\ell+1}g(x)) = \frac{(x_{n+k+1} + \ell)\square_{n+1}^{(k)}((x)_\ell g(x)) - (x_n + \ell)\square_n^{(k)}((x)_\ell g(x))}{x_{n+k+1} - x_n} \tag{B.1}$$

holds. The proof is based on the Leibniz formula for divided differences (see, e.g., [69, p. 50]) that yields upon use of $(x)_{\ell+1} = (x + \ell)(x)_\ell$ and $\square_n^{(k)}(x) = x_n \delta_{k,0} + \delta_{k,1}$

$$\begin{aligned} \square_n^{(k+1)}((x)_{\ell+1}g(x)) &= \ell \square_n^{(k+1)}((x)_\ell g(x)) + \sum_{j=0}^{k+1} \square_n^{(j)}(x) \square_{n+j}^{(k+1-j)}((x)_\ell g(x)) \\ &= (x_n + \ell) \square_n^{(k+1)}((x)_\ell g(x)) + \square_{n+1}^{(k)}((x)_\ell g(x)). \end{aligned} \tag{B.2}$$

Using the recursion relation of the divided differences, one obtains

$$\square_n^{(k+1)}((x)_{\ell+1}g(x)) = (x_n + \ell) \frac{\square_{n+1}^{(k)}((x)_\ell g(x)) - \square_n^{(k)}((x)_\ell g(x))}{x_{n+k+1} - x_n} + \square_{n+1}^{(k)}((x)_\ell g(x)). \tag{B.3}$$

Simple algebra then yields Eq. (B.1).

Comparison with Eq. (140) shows that using the interpolation conditions $g_n = g(x_n) = s_n/\omega_n$ and $\ell = k - 1$ in Eq. (B.1) yields the recursion for the numerators in Eq. (148), while the recursion for the denominators in Eq. (148) follows for $\ell = k - 1$ and using the interpolation conditions $g_n = g(x_n) = 1/\omega_n$. In each case, the initial conditions follow directly from Eq. (140) in combination with the definition of the divided difference operator: For $k = 0$, we use $(a)_{-1} = 1/(a - 1)$ and obtain $\square_n^{(k)}(x_n)_{k-1}g_n = (x_n)_{-1}g_n = g_n/(x_n - 1)$.

Appendix C. Two lemmata

Lemma C.1. *Define*

$$A = \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \frac{\zeta^{n+j}}{(n+j)^{r+1}}, \tag{C.1}$$

where ζ is a zero of multiplicity m of $\overset{\circ}{\Pi}^{(k)}(z) = \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} z^j$. Then

$$A \sim \zeta^{n+m} \binom{r+m}{r} \frac{(-1)^m}{n^{r+m+1}} \frac{d^m \overset{\circ}{\Pi}^{(k)}}{dx^m}(\zeta) \quad (n \rightarrow \infty). \tag{C.2}$$

Proof. Use

$$\frac{1}{a^{r+1}} = \frac{1}{r!} \int_0^\infty \exp(-at) t^r dt, \quad a > 0 \tag{C.3}$$

to obtain

$$A = \frac{1}{r!} \int_0^\infty \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} \zeta^{n+j} \exp(-(n+j)t) t^r dt = \frac{\zeta^n}{r!} \int_0^\infty \exp(-nt) \overset{\circ}{\Pi}^{(k)}(\zeta \exp(-t)) t^r dt. \tag{C.4}$$

Taylor expansion of the polynomial yields due to the zero at ζ

$$\overset{\circ}{\Pi}^{(k)}(\zeta \exp(-t)) = \frac{(-\zeta)^m}{m!} \left. \frac{d^m \overset{\circ}{\Pi}^{(k)}(x)}{dx^m} \right|_{x=\zeta} t^m (1 + O(t)). \tag{C.5}$$

Invoking Watson’s lemma [6, p. 263ff] completes the proof. \square

Lemma C.2. *Assume that assumption (C-3') of Theorem 13 holds. Further assume $\lambda_{n,j}^{(k)} \rightarrow \overset{\circ}{\lambda}_j^{(k)}$ for $n \rightarrow \infty$. Then, Eq. (280) holds.*

Proof. We have

$$\frac{\omega_{n+j}}{\omega_n} \sim \rho^j \exp\left(\varepsilon_n \sum_{t=0}^{j-1} \frac{\varepsilon_{n+t}}{\varepsilon_n}\right) \sim \rho^j \exp(j\varepsilon_n) \tag{C.6}$$

for large n . Hence,

$$\sum_{j=0}^k \lambda_{n,j}^{(k)} \frac{\omega_n}{\omega_{n+j}} \sim \sum_{j=0}^k \overset{\circ}{\lambda}_j^{(k)} (\rho \exp(\varepsilon_n))^{-j} = \overset{\circ}{\Pi}^{(k)}(1/\rho + \delta_n) \tag{C.7}$$

Since the characteristic polynomial $\overset{\circ}{\Pi}^{(k)}(z)$ has a zero of order μ at $z = 1/\rho$ according to the assumptions, Eq. (280) follows using Taylor expansion. \square

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Vector extrapolation methods. Applications and numerical comparison

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Abstract

The present paper is a survey of the most popular vector extrapolation methods such as the reduced rank extrapolation (RRE), the minimal polynomial extrapolation (MPE), the modified minimal polynomial extrapolation (MMPE), the vector ε -algorithm (VEA) and the topological ε -algorithm (TEA). Using projectors, we derive a different interpretation of these methods and give some theoretical results. The second aim of this work is to give a numerical comparison of the vector extrapolation methods above when they are used for practical large problems such as linear and nonlinear systems of equations. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Linear systems; Nonlinear systems; Extrapolation; Projection; Vector sequences; Minimal polynomial; Epsilon-algorithm

1. Introduction

In the last decade, many iterative methods for solving large and sparse nonsymmetric linear systems of equations have been developed. The extensions of these methods to nonlinear systems have been considered. As the classical iteration processes may converge slowly, extrapolation methods are required. The aim of vector extrapolation methods is to transform a sequence of vectors generated by some process to a new one with the goal to converge faster than the initial sequence. The most popular vector extrapolation methods can be classified into two categories: the polynomial methods and the ε -algorithms. The first family contains the minimal polynomial extrapolation (MPE) method of Cabay and Jackson [8], the reduced rank extrapolation (RRE) method of Eddy [9] and Mesina [24] and the modified minimal polynomial extrapolation (MMPE) method of Sidi et al. [35], Brezinski [3] and Pugachev [25]. The second class includes the topological ε -algorithm (TEA) of

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Brezinski [3] and the scalar and vector ε -algorithms (SEA and VEA) of Wynn [39,40]. Some convergence results and properties of these methods were given in [3,16,18,28,30,33–36].

Different recursive algorithms for implementing these methods were also proposed in [5,15,10,39,40]. However, in practice and for large problems, these algorithms become very unstable and are not recommended. When solving large linear and nonlinear systems, Sidi [32] gives a more stable implementation of the RRE and MPE methods using a QR decomposition while Jbilou and Sadok [19] developed an LU-implementation of the MMPE method. These techniques require low storage and work and are more stable numerically.

When applied to linearly generated vector sequences, the MPE, the RRE and the TEA methods are mathematically related to some known Krylov subspace methods. It was shown in [34] that these methods are equivalent to the method of Arnoldi [26], the generalized minimal residual method (GMRES) [27] and the method of Lanczos [21], respectively. The MMPE method is mathematically equivalent to Hessenberg method [30] and [38]. For linear problems, some numerical comparisons have been given in [11].

We note also that, when the considered sequence is not generated linearly, these extrapolation methods are still projection methods but not necessarily Krylov subspace methods [20].

An important property of the vector extrapolation methods above is that they could be applied directly to the solution of linear and nonlinear systems. This comes out from the fact that the definitions of these methods do not require an explicit knowledge of how the sequence is generated. Hence, these vector extrapolation methods are more effective for nonlinear problems [29].

For nonlinear problems, these methods do not need the use of the Jacobian of the function and have the property of quadratic convergence under some assumptions [17]. Note that for some nonlinear problems, vector extrapolation methods such as nonlinear Newton–Krylov methods fail to converge if the initial guess is “away” from a solution. In this case, some techniques such as the linear search backtracking procedure could be added to the basic algorithms; see [2].

The paper is organized as follows. In Section 2, we introduce the polynomial extrapolation methods (RRE, MPE and MMPE) by using the generalized residual. We will also see how these methods could be applied for solving linear and nonlinear systems of equations. In this case some theoretical results are given. Section 3 is devoted to the epsilon-algorithm’s family (SEA, VEA and TEA). In Section 4, we give the computational steps and storage required for these methods. Some numerical experiments are given in Section 5 and a comparison with the vector extrapolation methods cited above.

In this paper, we denote by $(.,.)$ the Euclidean inner product in \mathbb{R}^N and by $\|.\|$ the corresponding norm. For an $N \times N$ matrix A and a vector v of \mathbb{R}^N the Krylov subspace $K_k(A, v)$ is the subspace generated by the vectors $v, Av, \dots, A^{k-1}v$. I_N is the unit matrix and the Kronecker product \otimes is defined by $C \otimes B = [c_{i,j} B]$ where B and C are two matrices.

2. The polynomial methods

2.1. Definitions of the RRE, MPE and MMPE methods

Let (s_n) be a sequence of vectors of \mathbb{R}^N and consider the transformation T_k defined by

$$\begin{aligned} T_k : \mathbb{R}^N &\rightarrow \mathbb{R}^N, \\ s_n &\rightarrow t_k^{(n)} \end{aligned}$$

with

$$t_k^{(n)} = s_n + \sum_{i=1}^k a_i^{(n)} g_i(n), \quad n \geq 0, \tag{2.1}$$

where the auxiliary vector sequences $(g_i(n))_n; i = 1, \dots, k$, are given. The coefficients $a_i^{(n)}$ are scalars.

Let \tilde{T}_k denote the new transformation obtained from T_k by

$$\tilde{t}_k^{(n)} = s_{n+1} + \sum_{i=1}^k a_i^{(n)} g_i(n+1), \quad n \geq 0. \tag{2.2}$$

For these extrapolation methods, the auxiliary sequences are such that $g_i(n) = \Delta s_{n+i-1}, i = 1, \dots, k; n \geq 0$, and the coefficients $a_i^{(n)}$ are the same in the two expressions (2.1) and (2.2).

We define the generalized residual of $t_k^{(n)}$ by

$$\begin{aligned} \tilde{r}(t_k^{(n)}) &= \tilde{t}_k^{(n)} - t_k^{(n)} \\ &= \Delta s_n + \sum_{i=1}^k a_i^{(n)} \Delta g_i(n). \end{aligned} \tag{2.3}$$

The forward difference operator Δ acts on the index n , i.e., $\Delta g_i(n) = g_i(n+1) - g_i(n), i = 1, \dots, k$.

We will see later that, when solving linear systems of equations, the sequence $(s_n)_n$ is generated by a linear process and then the generalized residual coincides with the classical residual.

The coefficients $a_i^{(n)}$ involved in expression (2.1) are obtained from the orthogonality relation

$$\tilde{r}(t_k^{(n)}) \perp \text{span}\{y_1^{(n)}, \dots, y_k^{(n)}\}, \tag{2.4}$$

where $y_i^{(n)} = \Delta s_{n+i-1}$ for the MPE; $y_i^{(n)} = \Delta^2 s_{n+i-1}$ for the RRE and $y_i^{(n)} = y_i$ for the MMPE where y_1, \dots, y_k are arbitrary linearly independent vectors of \mathbb{R}^N .

Now, if $\tilde{W}_{k,n}$ and $\tilde{L}_{k,n}$ denote the subspaces $\tilde{W}_{k,n} = \text{span}\{\Delta^2 s_n, \dots, \Delta^2 s_{n+k-1}\}$ and $\tilde{L}_{k,n} = \text{span}\{y_1^{(n)}, \dots, y_k^{(n)}\}$, then from (2.3) and (2.4), the generalized residuals satisfies

$$\tilde{r}(t_k^{(n)}) - \Delta s_n \in \tilde{W}_{k,n} \tag{2.5}$$

and

$$\tilde{r}(t_k^{(n)}) \perp \tilde{L}_{k,n}. \tag{2.6}$$

Conditions (2.5) and (2.6) show that the generalized residual $\tilde{r}(t_k^{(n)})$ is obtained by projecting, the vector Δs_n onto the subspace $\tilde{W}_{k,n}$, orthogonally to $\tilde{L}_{k,n}$.

In a matrix form, $\tilde{r}(t_k^{(n)})$ can be written as

$$\tilde{r}(t_k^{(n)}) = \Delta s_n - \Delta^2 S_{k,n} (L_{k,n}^T \Delta^2 S_{k,n})^{-1} L_{k,n}^T \Delta s_n, \tag{2.7}$$

where $L_{k,n}, \Delta S_{k,n}$ and $\Delta^2 S_{k,n}$ are the $k \times k$ matrices whose columns are $y_1^{(n)}, \dots, y_k^{(n)}, \Delta s_n, \dots, \Delta s_{n+k-1}$ and $\Delta^2 s_n, \dots, \Delta^2 s_{n+k-1}$ respectively. Note that $\tilde{r}(t_k^{(n)})$ is well defined if and only if the $k \times k$ matrix

$L_{k,n}^T \Delta^2 S_{k,n}$ is nonsingular; a necessary condition for this is that the matrices $L_{k,n}$ and $\Delta^2 S_{k,n}$ are full rank. In this case, $t_k^{(n)}$ exists and is uniquely given by

$$t_k^{(n)} = s_n - \Delta S_{k,n} (L_{k,n}^T \Delta^2 S_{k,n})^{-1} L_{k,n}^T \Delta s_n. \tag{2.8}$$

The approximation $t_k^{(n)}$ can also be expressed as

$$t_k^{(n)} = \sum_{j=0}^k \beta_j^{(n)} s_{n+j}$$

with

$$\sum_{i=0}^k \beta_i^{(n)} = 1$$

and

$$\sum_{j=0}^k \alpha_{i,j}^{(n)} \beta_j^{(n)} = 0, \quad j = 0, \dots, k - 1,$$

where the coefficients $\alpha_{i,j}^{(n)}$ are defined by

$$\begin{aligned} \alpha_{i,j}^{(n)} &= (\Delta s_{n+i}, \Delta s_{n+j}) \quad \text{for the MPE method,} \\ \alpha_{i,j}^{(n)} &= (\Delta^2 s_{n+i}, \Delta s_{n+j}) \quad \text{for the RRE method,} \\ \alpha_{i,j}^{(n)} &= (y_{i+1}, \Delta s_{n+j}) \quad \text{for the MPE method, } i = 0, \dots, k - 1 \text{ and } j = 0, \dots, k. \end{aligned}$$

From these relations it is not difficult to see that $t_k^{(n)}$ can also be written as a ratio of two determinants as follows:

$$t_k^{(n)} = \frac{\begin{vmatrix} s_n & s_{n+1} & \dots & s_{n+k} \\ \alpha_{0,0}^{(n)} & \alpha_{0,1}^{(n)} & \dots & \alpha_{0,k}^{(n)} \\ \vdots & \vdots & & \vdots \\ \alpha_{k-1,0}^{(n)} & \alpha_{k-1,1}^{(n)} & \dots & \alpha_{k-1,k}^{(n)} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \dots & 1 \\ \alpha_{0,0}^{(n)} & \alpha_{0,1}^{(n)} & \dots & \alpha_{0,k}^{(n)} \\ \vdots & \vdots & & \vdots \\ \alpha_{k-1,0}^{(n)} & \alpha_{k-1,1}^{(n)} & \dots & \alpha_{k-1,k}^{(n)} \end{vmatrix}}. \tag{2.9}$$

The determinant in the numerator of (2.9) is the vector obtained by expanding this determinant with respect to its first row by the classical rule.

Note that the determinant in the denominator of (2.9) is equal to $\det(L_{k,n}^T \Delta^2 S_{k,n})$ which is assumed to be nonzero. The computation of the approximation $t_k^{(n)}$ needs the values of the terms $s_n, s_{n+1}, \dots, s_{n+k+1}$.

2.2. Application to linear systems

Consider the system of linear equations

$$Cx = f, \tag{2.10}$$

where C is a real nonsingular $N \times N$ matrix, f is a vector of \mathbb{R}^N and x^* denotes the unique solution.

Instead of applying the extrapolation methods for solving (2.10), we will use them for the pre-conditioned linear system

$$M^{-1}Cx = M^{-1}f, \tag{2.11}$$

where M is a nonsingular matrix.

Starting from an initial vector s_0 , we construct the sequence $(s_j)_j$ by

$$s_{j+1} = Bs_j + b; \quad j = 0, 1, \dots \tag{2.12}$$

with $B = I - A$; $A = M^{-1}C$ and $b = M^{-1}f$.

Note that if the sequence (s_j) is convergent, its limit $s = x^*$ is the solution of the linear system (2.10).

From (2.12) we have $\Delta s_j = b - As_j = r(s_j)$, the residual of the vector s_j . Therefore using (2.3) and (2.12), it follows that the generalized residual of the approximation $t_k^{(n)}$ is the true residual

$$\tilde{r}(t_k^{(n)}) = r(t_k^{(n)}) = b - At_k^{(n)}. \tag{2.13}$$

Note also that, since $\Delta^2 s_n = -A\Delta s_n$, we have $\Delta^2 S_{k,n} = -A\Delta S_{k,n}$.

For simplicity and unless specified otherwise, we set $n = 0$, we denote $t_k^{(0)} = t_k$ and we drop the index n in our notations. Let d be the degree of the minimal polynomial \mathcal{P}_d of B for the vector $s_0 - x^*$ and, as $A = I - B$ is nonsingular, P_d is also the minimal polynomial of B for $r_0 = \Delta s_0$. Therefore, the matrices $\Delta S_k = [\Delta s_0, \dots, \Delta s_{k-1}]$ and $\Delta^2 S_k = [\Delta^2 s_0, \dots, \Delta^2 s_{k-1}]$ have full rank for $k \leq d$. We also note that the approximation t_d exists and is equal to the solution of the linear system (2.10).

The three extrapolation methods make use implicitly of the polynomial \mathcal{P}_d and since this polynomial is not known in practice, the aim of these methods is to approximate it.

When applied to the sequence generated by (2.12), the vector extrapolation methods above produce approximations t_k such that the corresponding residuals $r_k = b - At_k$ satisfy the relations

$$r_k \in \tilde{W}_k = A\tilde{V}_k \tag{2.14}$$

and

$$r_k \perp \tilde{L}_k, \tag{2.15}$$

where $\tilde{V}_k = \text{span}\{\Delta s_0, \dots, \Delta s_{k-1}\}$ and $\tilde{L}_k \equiv \tilde{W}_k$ for RRE, $\tilde{L}_k \equiv \tilde{V}_k$ for MPE and $\tilde{L}_k \equiv \tilde{Y}_k = \text{span}\{y_1, \dots, y_k\}$ for MMPE where y_1, \dots, y_k are linearly independent vectors.

Note that, since $\tilde{W}_k \equiv K_k(A, Ar_0)$, the extrapolation methods above are Krylov subspace methods. RRE is an orthogonal projection and is theoretically equivalent to GMRES while MPE and MMPE are oblique projection methods and are equivalent to the method of Arnoldi and to the Hessenberg method [38], respectively. From this observation, we conclude that for $k \leq d$, the approximation t_k exists and is unique, unconditionally for RRE, and this is not always the case for MPE and MMPE. In fact, for the last two methods the approximation t_k ($k < d$) exists if and only if $\det(\Delta S_k^T \Delta^2 S_k) \neq 0$ for MPE and $\det(Y_k^T \Delta^2 S_k) \neq 0$ for MMPE where $Y_k = [y_1, \dots, y_k]$.

Let P_k be the orthogonal projector onto \tilde{W}_k . Then from (2.14) and (2.15), the residual generated by RRE can be expressed as

$$r_k^{\text{rre}} = r_0 - P_k r_0. \tag{2.16}$$

We also consider the oblique projectors Q_k and R_k onto \tilde{W}_k and orthogonally to \tilde{V}_k and \tilde{Y}_k respectively. It follows that the residuals produced by MPE and MMPE can be written as

$$r_k^{\text{mpe}} = r_0 - Q_k r_0 \tag{2.17}$$

and

$$r_k^{\text{mmpe}} = r_0 - R_k r_0. \tag{2.18}$$

The acute angle θ_k between r_0 and the subspace \tilde{W}_k is defined by

$$\cos \theta_k = \max_{z \in \tilde{W}_k - \{0\}} \left(\frac{|(r_0, z)|}{\|r_0\| \|z\|} \right). \tag{2.19}$$

Note that θ_k is the acute angle between the vector r_0 and $P_k r_0$.

In the sequel we give some relations satisfied by the residual norms of the three extrapolation methods.

Theorem 1. *Let ϕ_k be the acute angle between r_0 and $Q_k r_0$ and let ψ_k denote the acute angle between r_0 and $R_k r_0$. Then we have the following relations:*

- (1) $\|r_k^{\text{rre}}\|^2 = (\sin^2 \theta_k) \|r_0\|^2.$
- (2) $\|r_k^{\text{mpe}}\|^2 = (\tan^2 \phi_k) \|r_0\|^2.$
- (3) $\|r_k^{\text{rre}}\| \leq (\cos \phi_k) \|r_k^{\text{mpe}}\|.$

Moreover if for MMPE $y_j = r_0$ for some $j = 1, \dots, k$, then we also have

- (4) $\|r_k^{\text{mmpe}}\|^2 = (\tan^2 \psi_k) \|r_0\|^2.$
- (5) $\|r_k^{\text{rre}}\| \leq (\cos \psi_k) \|r_k^{\text{mmpe}}\|.$

Proof. Parts (1)–(3) have been proved in [18]

(4) From (2.18), we get

$$(r_k^{\text{mmpe}}, r_k^{\text{mmpe}}) = (r_k^{\text{mmpe}}, r_0 - R_k r_0).$$

Since $(r_k^{\text{mmpe}}, r_0) = 0$, it follows that

$$\begin{aligned} (r_k^{\text{mmpe}}, r_k^{\text{mmpe}}) &= (r_k^{\text{mmpe}}, -R_k r_0) \\ &= -\|r_k^{\text{mmpe}}\| \|R_k r_0\| \cos(r_k^{\text{mmpe}}, R_k r_0) \\ &= \|r_k^{\text{mmpe}}\| \|R_k r_0\| \sin \psi_k. \end{aligned}$$

On the other hand,

$$\|r_0\| = \|R_k r_0\| \cos \psi_k,$$

hence

$$\|r_k^{\text{mmpe}}\| = \|r_0\| \tan \psi_k.$$

(5) Using statements (1) and (4), we get

$$\frac{\|r_k^{\text{mmpe}}\|^2}{\|r_k^{\text{rre}}\|^2} = \frac{1 - \cos^2 \psi_k}{1 - \cos^2 \theta_k} (\cos^2 \psi_k)^{-1}.$$

But $\cos \psi_k \leq \cos \theta_k$, therefore

$$\|r_k^{\text{rre}}\| \leq \|r_k^{\text{mmpe}}\| \cos \psi_k. \quad \square$$

Remark.

- From relations (1), (2) and (4) of Theorem 1, we see that the residuals of the RRE are always defined while those produced by MPE and MMPE may not exist.
- We also observe that if a stagnation occurs in RRE ($\|r_k^{\text{rre}}\| = \|r_0\|$ for some $k < d$), then $\cos \theta_k = 0$ and, from (2.19), this implies that $\cos \phi_k = \cos \psi_k = 0$ and hence the approximations produced by MPE and MMPE are not defined.

When the linear process (2.12) is convergent, it is more useful in practice to apply the extrapolation methods after a fixed number p of basic iterations. We note also that, when these methods are used in their complete form, the required work and storage grow linearly with the iteration step. To overcome this drawback we use them in a cycling mode and this means that we have to restart the algorithms after a chosen number m of iterations.

The algorithm is summarized as follows:

1. $k = 0$, choose x_0 and the numbers p and m .
2. Basic iteration
 - set $t_0 = x_0$
 - $z_0 = t_0$
 - $z_{j+1} = Bz_j + b, j = 0, \dots, p - 1.$
3. Extrapolation scheme
 - $s_0 = z_p$
 - $s_{j+1} = Bs_j + b, j = 0, \dots, m,$
 - compute the approximation t_m by RRE, MPE or MMPE.
4. Set $x_0 = t_m, k = k + 1$ and go to 2.

Stable schemes for the computation of the approximation t_k are given in [32, 19]. In [32], Sidi gave an efficient implementation of the MPE and RRE methods which is based on the QR decomposition of the matrix ΔS_k . In [19], we used an LU decomposition of ΔS_k with a pivoting strategy. These implementations require low work and storage and are more stable numerically.

2.3. Application to nonlinear systems

Consider the system of nonlinear equations

$$G(x) = x, \tag{2.20}$$

where $G: \mathbb{R}^N \Rightarrow \mathbb{R}^N$ and let x^* be a solution of (2.20).

For any arbitrary vector x , the residual is defined by

$$r(x) = G(x) - x.$$

Let $(s_j)_j$ be the sequence of vectors generated from an initial guess s_0 as follows:

$$s_{j+1} = G(s_j), \quad j = 0, 1, \dots \tag{2.21}$$

Note that

$$r(s_j) = \tilde{r}(s_j) = \Delta s_j, \quad j=, 1, \dots .$$

As for linear problems, it is more useful to run some basic iterations before the application of an extrapolation method for solving (2.20). Note also that the storage and the evaluation of the function G increase with the iteration step k . So, in practice, it is recommended to restart the algorithms after a fixed number of iterations. Another important remark is the fact that the extrapolation methods are more efficient if they are applied to a preconditioned nonlinear system

$$\tilde{G}(x) = x, \tag{2.22}$$

where the function \tilde{G} is obtained from G by some preconditioning nonlinear technique.

An extrapolation algorithm for solving the nonlinear problem (2.22) is summarized as follows:

1. $k = 0$, choose x_0 and the integers p and m .
2. Basic iteration
 - set $t_0 = x_0$
 - $w_0 = t_0$
 - $w_{j+1} = \tilde{G}(w_j), j = 0, \dots, p - 1.$
3. Extrapolation phase
 - $s_0 = w_p;$
 - if $\|s_1 - s_0\| < \varepsilon$ stop;
 - otherwise generate $s_{j+1} = \tilde{G}(s_j), j = 0, \dots, m,$
 - compute the approximation t_m by RRE, MPE or MMPE;
4. set $x_0 = t_m, k = k + 1$ and go to 2.

As for systems of linear equations, efficient computation of the approximation t_m produced by RRE, MPE and MMPE have been derived in [32,19]. These implementations give as an estimation of the residual norm at each iteration and it allows to stop the algorithms without having to compute the true residual which requires an extra evaluation of the function \tilde{G} .

Important properties of vector extrapolation methods is the fact that they do not use the knowledge of the Jacobian of the function \tilde{G} and have a quadratic convergence (when they are used in their complete form).

We also note that the results of Theorem 1 are still valid for nonlinear problems by replacing in the relations of this theorem the residual r_k by the generalized residual \tilde{r}_k .

Vector extrapolation methods such as MMPE can also be used for computing eigenelements of a matrix [16].

3. The ε -algorithms

3.1. The scalar ε -algorithm

Let (x_n) be a scalar sequence and consider the Hankel determinant

$$H_k(x_n) = \begin{vmatrix} x_n & \dots & x_{n+k-1} \\ \vdots & \vdots & \vdots \\ x_{n+k-1} & \dots & x_{n+2k-2} \end{vmatrix}, \quad \text{with } H_0(x_n) = 0, \quad \forall n.$$

Shanks’s transformation [31] e_k is defined by

$$e_k(x_n) = \frac{H_{k+1}(x_n)}{H_k(\Delta^2 x_n)}. \tag{3.1}$$

For the kernel of the transformation e_k , it was proved (see [6]) that

$$\forall n, e_k(x_n) = x \Leftrightarrow \exists a_0, \dots, a_k \text{ with } a_k \neq 0 \text{ and } a_0 + \dots + a_k \neq 0 \text{ such that } \forall n, \sum_{i=0}^k a_i(x_{n+i} - x) = 0.$$

To implement Shank’s transformation without computing determinants, Wynn [39] discovered a simple recursion called the scalar epsilon algorithm (SEA) defined by

$$\begin{aligned} \varepsilon_{-1}^{(n)} &= 0, \quad \varepsilon_0^{(n)} = x_n, \quad n = 0, 1, \dots, \\ \varepsilon_{k+1}^{(n)} &= \varepsilon_{k-1}^{(n+1)} + \frac{1}{\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}} k, \quad n = 0, 1, \dots \end{aligned}$$

The scalar ε -algorithm is related to Shanks’s transformation by

$$\varepsilon_{2k}^{(n)} = e_k(x_n) \quad \text{and} \quad \varepsilon_{2k+1}^{(n)} = \frac{1}{e_k(\Delta x_n)}.$$

For more details and properties of SEA, see [6] and the references therein. For vector sequences (s_n) , one can apply the scalar ε -algorithm to each component of s_n . However, one disadvantage of this technique is that it ignores the connexions between the components. Another problem is the fact that some transformed components fail to exist or may be very large numerically. These drawbacks limit the application of SEA to vector sequences.

3.2. The vector ε -algorithm

In order to generalize the scalar ε -algorithm to the vector case, we have to define the inverse of a vector. One possibility that was considered by Wynn [40] is to use the inverse defined by

$$z^{-1} = \frac{z}{\|z\|^2}, \quad z \in \mathbb{R}^N.$$

Therefore, for vector sequences (s_n) the vector ε -algorithm of Wynn is defined by

$$\begin{aligned} \varepsilon_{-1}^{(n)} &= 0, \quad \varepsilon_0^{(n)} = s_n, \quad n = 0, 1, \dots, \\ \varepsilon_{k+1}^{(n)} &= \varepsilon_{k-1}^{(n+1)} + [\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}]^{-1}, \quad k, n = 0, 1, \dots \end{aligned}$$

For the real case, it was proved by McLeod [23] that if $\forall n \geq N_0, \sum_{i=0}^k a_i(s_{n+i} - s) = 0$, with $a_k \neq 0$ and $a_0 + \dots + a_k \neq 0$, then $\varepsilon_{2k}^{(n)} = s; \forall n \geq N_0$. This result has been proved by Graves-Morris [13] in the complex case.

When applied to the vector sequence generated by (2.12), the scalar and the vector ε -algorithms give the solution of the linear system (2.10) that is $\forall n, \varepsilon_{2N}^{(n)} = x^*$, see [6]. As will be seen in the last section, the intermediate quantities $\varepsilon_{2k}^{(n)}, k < N$, are approximations of the solution x^* .

We note also that the vector ε -algorithm has been used for solving nonlinear problems by applying it to the nonlinear sequence defined by (2.21); see [7,12].

However, the vector ε -algorithm requires higher work and storage as compared to the vector polynomial methods described in Section 2. In fact, computing the approximation $\varepsilon_{2k}^{(n)}$ needs the terms s_n, \dots, s_{n+2k} which requires a storage of $2k + 1$ vectors of \mathbb{R}^N while the three methods (RRE, MPE and MMPE) require only $k + 2$ terms s_n, \dots, s_{n+k+1} . Computational work and storage requirements are given in Section 4.

3.3. The topological ε -algorithm

In [3], Brezinski proposed another generalization of the scalar ε -algorithm for vector sequences which is quite different from the vector ε -algorithm and was called the topological ε -algorithm (TEA).

This approach consists in computing approximations $e_k(s_n) = t_k^{(n)}$ of the limit or the anti-limit of the sequence (s_n) such that

$$t_k^{(n)} = s_n + \sum_{i=1}^k a_i^{(n)} \Delta s_{n+i-1}, \quad n \geq 0. \tag{3.2}$$

We consider the new transformations $\tilde{t}_{k,j}, j = 1, \dots, k$ defined by

$$\tilde{t}_{k,j}^{(n)} = s_{n+j} + \sum_{i=1}^k a_i^{(n)} \Delta s_{n+i+j-1}, \quad j = 1, \dots, k.$$

We set $\tilde{t}_{k,0}^{(n)} = t_k^{(n)}$ and define the j th generalized residual as follows:

$$\begin{aligned} \tilde{r}_j(t_k^{(n)}) &= \tilde{t}_{k,j}^{(n)} - \tilde{t}_{k,j-1}^{(n)} \\ &= \Delta s_{n+j-1} + \sum_{i=1}^k a_i^{(n)} \Delta^2 s_{n+i+j-2}, \quad j = 1, \dots, k. \end{aligned}$$

Therefore, the coefficients involved in expression (3.2) of $t_k^{(n)}$ are computed such that each j th generalized residual is orthogonal to some chosen vector $y \in \mathbb{R}^N$, that is

$$(y, \tilde{r}_j(t_k^{(n)})) = 0, \quad j = 1, \dots, k. \tag{3.3}$$

Hence the vector $a_n = (a_1^{(n)}, \dots, a_k^{(n)})^T$ is the solution of the $k \times k$ linear system (3.3) which is written as

$$T_{k,n} a_n = \Delta S_{k,n}^T y, \tag{3.4}$$

where $T_{k,n}$ is the matrix whose columns are $\Delta^2 S_{k,n}^T y, \dots, \Delta^2 S_{k,n+k-1}^T y$ (assumed to be nonsingular) and $\Delta^j S_{k,n}, j = 1, 2$ are the $N \times k$ matrices whose columns are $\Delta^j s_n, \dots, \Delta^j s_{n+k-1}, j = 1, 2$.

Note that the $k \times k$ matrix $T_{k,n}$ is also given by the formula

$$T_{k,n} = \mathcal{S}_{k,n} (I_N \otimes y),$$

where $\mathcal{S}_{k,n}$ is the $k \times Nk$ matrix whose block columns are $\Delta^2 S_{k,n}^T, \dots, \Delta^2 S_{k,n+k-1}^T$.

Invoking (3.2) and (3.4), $t_k^{(n)}$ can be expressed in a matrix form as

$$t_k^{(n)} = s_n - \Delta S_{k,n} T_{k,n}^{-1} \Delta S_{k,n}^T y. \tag{3.5}$$

Using Schur’s formula, $t_k^{(n)}$ can be expressed as a ratio of two determinants

$$t_k^{(n)} = \left| \begin{array}{cc} s_n & \Delta S_{k,n} \\ \Delta S_{k,n}^T y & T_{k,n} \end{array} \right| / \det(T_{k,n}).$$

For the kernel of the topological ε -algorithm it is easy to see that if $\forall n, \exists a_0, \dots, a_k$ with $a_k \neq 0$ and $a_0 + \dots + a_k \neq 0$ such that $\sum_{i=0}^k a_i (s_{n+i} - s) = 0$, then $\forall n, t_k^{(n)} = s$.

The vectors $e_k(s_n) = t_k^{(n)}$ can be recursively computed by the topological ε -algorithm discovered by Brezinski [3]

$$\begin{aligned} \varepsilon_{-1}^{(n)} &= 0; \quad \varepsilon_0^{(n)} = s_n, \quad n = 0, 1, \dots, \\ \varepsilon_{2k+1}^{(n)} &= \varepsilon_{2k-1}^{(n+1)} + \frac{y}{(y, \Delta \varepsilon_{2k}^{(n)})}, \\ \varepsilon_{2k+2}^{(n)} &= \varepsilon_{2k}^{(n+1)} + \frac{\Delta \varepsilon_{2k}^{(n)}}{(\Delta \varepsilon_{2k+1}^{(n)}, \Delta \varepsilon_{2k}^{(n)})} n, \quad k = 0, 1, \dots \end{aligned}$$

The forward difference operator Δ acts on the superscript n and we have

$$\varepsilon_{2k}^{(n)} = e_k(s_n) = t_k^{(n)}, \quad \text{and} \quad \varepsilon_{2k+1}^{(n)} = \frac{y}{(y, e_k(\Delta s_n))}, \quad n, k = 0, 1, \dots$$

We notice that, for the complex case, we can use the product $(y, z) = \sum_{i=1}^N y_i \bar{z}_i$, hence (y, z) is not equal to (z, y) . The order of vectors in the scalar product is important, and similar methods have been studied in detail by Tan [37].

3.4. Application of VEA and TEA to linear and nonlinear systems

Consider again the system of linear equations (2.10) and let (s_n) be the sequence of vectors generated by the linear process (2.12).

Using the fact that $\Delta^2 s_{n+i} = B \Delta^2 s_{n+i-1}$, the matrix $T_{k,n}$ has now the following expression:

$$T_{k,n} = -L_k^T A \Delta S_{k,n}, \tag{3.6}$$

where L_k is the $N \times k$ matrix whose columns are $y, B^T y, \dots, B^{T^{k-1}} y$. As n will be a fixed integer, we set $n = 0$ for simplicity and denote $T_{k,0}$ by T_k and $\Delta S_{k,0}$ by ΔS_k .

On the other hand, it is not difficult to see that

$$\Delta S_k^T y = L_k^T r_0. \tag{3.7}$$

Therefore, using (3.6), (3.7) with (3.5), the k th residual produced by TEA is given by

$$r_k^{\text{tea}} = r_0 - A \Delta S_k (L_k^T A \Delta S_k)^{-1} L_k^T r_0. \tag{3.8}$$

Let E_k denotes the oblique projector onto the Krylov subspace $K_k(A, Ar_0)$ and orthogonally to the Krylov subspace $K_k(B^T, y) = K_k(A^T, y)$. Then from (3.8) the residual generated by TEA can be written as follows:

$$r_k^{\text{tea}} = r_0 - E_k r_0. \tag{3.9}$$

This shows that the topological ε -algorithm is mathematically equivalent to the method of Lanczos [4]. Note that the k th approximation defined by TEA exists if and only if the $k \times k$ matrix $L_k^T A \Delta S_k$ is nonsingular.

The following result gives us some relations satisfied by the residual norms in the case where $y = r_0$.

Theorem 2. *Let φ_k be the acute angle between r_0 and $E_k r_0$ and let $y = r_0$. Then we have the following relations:*

- (1) $\|r_k^{\text{tea}}\| = |\tan \varphi_k| \|r_0\|; k > 1.$
- (2) $\|r_k^{\text{rre}}\| \leq (\cos \varphi_k) \|r_k^{\text{tea}}\|.$

Proof. (1) Follows from (3.9) and the fact that $r_0 = y$ is orthogonal to r_k^{tea} .

(2) From (2.19) we have $\cos \varphi_k \leq \cos \theta_k$, then using relations (1) of Theorem 1 and (1) of Theorem 2 the result follows. \square

Remark.

- Relation (1) of Theorem 2 shows that the residuals of the TEA are defined if and only if $\cos \varphi_k \neq 0$.
- We also observe that, if a stagnation occurs in RRE ($\|r_k^{\text{rre}}\| = \|r_0\|$ for some k , then $\cos \theta_k = 0$ and this implies that $\cos \varphi_k = 0$, which shows that the TEA-approximation is not defined.

The topological ε -algorithm can also be applied for solving nonlinear systems of equations. For this, TEA is applied to the sequence (s_n) generated by the nonlinear process (2.22). We note that TEA does not need the knowledge of the Jacobian of the function \tilde{G} and has the property of quadratic convergence [22].

When applied for the solution of linear and nonlinear problems, work and storage required by VEA and TEA grow with the iteration step. So, in practice and for large problems, the algorithms must be restarted. It is also useful to run some basic iterations before the extrapolation phase.

The application of VEA or TEA for linear and nonlinear systems leads to the following algorithm where $\tilde{G}(x)$ is to be replaced by $Bx + b$ for linear problems:

1. $k = 0$, choose x_0 and the integers p and m .
2. Basic iteration
 - set $t_0 = x_0$
 - $w_0 = t_0$
 - $w_{j+1} = \tilde{G}(w_j), j = 0, \dots, p - 1.$
3. Extrapolation phase
 - $s_0 = w_p;$
 - if $\|s_1 - s_0\| < \varepsilon$ stop;
 - otherwise generate $s_{j+1} = \tilde{G}(s_j), j = 0, \dots, 2m - 1,$
 - compute the approximation $t_m = \varepsilon_{2m}^{(0)}$ by VEA or TEA;
4. set $x_0 = t_m, k = k + 1$ and go to 2.

Table 1

Memory requirements and computational costs (multiplications and additions) for RRE, MPE, MMPE, VEA and TEA

Method	RRE	MPE	MMPE	VEA	TEA
Multiplications and additions	$2Nk^2$	$2Nk^2$	Nk^2	$10Nk^2$	$10Nk^2$
Mat–Vec with A or evaluation of \tilde{G}	$k + 1$	$k + 1$	$k + 1$	$2k$	$2k$
Memory locations	$(k + 1)N$	$(k + 1)N$	$(k + 1)N$	$(2k + 1)N$	$(2k + 1)N$

4. Operation count and storage

Table 1 lists the operation count (multiplications and additions) and the storage requirements to compute the approximation $t_k^{(0)}$ with RRE, MPE and MMPE and the approximation $\varepsilon_{2k}^{(0)}$ with VEA and TEA. In practice, the dimension N of vectors is very large and k is small, so we listed only the main computational effort.

For RRE and MPE, we used the QR-implementation given in [32], whereas the LU-implementation developed in [19] was used for MMPE.

To compute $t_k^{(0)}$ with the three polynomial vector extrapolation methods, the vectors s_0, s_1, \dots, s_{k+1} are required while the terms s_0, \dots, s_{2k} are needed for the computation of $\varepsilon_{2k}^{(0)}$ with VEA and TEA. So, when solving linear systems of equations, $k + 1$ matrix–vector (Mat–Vec) products are required with RRE, MPE and MMPE and $2k$ matrix–vector products are needed with VEA and TEA. For nonlinear problems the comparison is still valid by replacing “Mat–Vec” with “evaluation of the function \tilde{G} ”.

All these operations are listed in Table 1.

As seen in Table 1, the vector and topological ε -algorithms are more expensive in terms of work and storage as compared to the polynomial vector extrapolation methods, namely RRE, MPE and MMPE.

The implementations given in [32,19] for RRE, MPE and MMPE allow us to compute exactly the norm of the residual at each iteration for linear systems or to estimate it for nonlinear problems without actually computing the residuals. This reduce the cost of implementation and is used to stop the algorithms when the accuracy is achieved.

5. Numerical examples

We report in this section a few numerical examples comparing the performances of RRE, MPE, MMPE, VEA and TEA. For RRE and MPE, we used the program given in [32] and for MMPE we used the implementation developed in [19]. The programs used for VEA and TEA were taken out from [6].

The tests were run in double precision on SUN Entreprise 450 SERVER using the standard F77 compiler. We have first considered one example for linear systems and one example for nonlinear systems. In these examples the starting point was chosen $x_0 = \text{rand}(N, 1)$ where the function rand creates an N vector with coefficients uniformly distributed in $[0, 1]$.

For the TEA the vector y was also $y = \text{rand}(N, 1)$.

Table 2

Method	MMPE	MPE	RRE	VEA	TEA
Number of restarts	28	25	26	30	30
Residual norms	2.16d-09	2.d-09	1.d-09	9d-04	3d-01
CPU time	40	80	83	230	206

5.1. Example 1

In the first example, we derived the matrix test problem by discretizing the boundary value problem [1]

$$-u_{xx}(x, y) - u_{yy}(x, y) + 2p_1u_x(x, y) + 2p_2u_y(x, y) - p_3u(x, y) = \phi(x, y) \quad \text{on } \Omega,$$

$$u(x, y) = 1 + xy \quad \text{on } \partial\Omega,$$

by finite differences, where Ω is the unit square $\{(x, y) \in R^2, 0 \leq x, y \leq 1\}$ and p_1, p_2, p_3 are positive constants. The right-hand-side function $\phi(x, y)$ was chosen so that the true solution is $u(x, y) = 1 + xy$ in Ω . We used centred differences to discretize this problem on a uniform $(n + 2) \times (n + 2)$ grid (including grid points on the boundary). We get a matrix of size $N = n^2$.

We applied the extrapolation methods to the sequence (s_j) defined as in [14] by

$$s_{j+1} = B_\omega s_k + c_\omega, \tag{5.1}$$

where

$$c_\omega = \omega(2 - \omega)(D - \omega U)^{-1}D(D - \omega L)^{-1}b, \tag{5.2}$$

$$B_\omega = (D - \omega U)^{-1}(\omega L + (1 - \omega)D)(D - \omega L)^{-1}(\omega U + (1 - \omega)D) \tag{5.3}$$

and $A = D - L - U$, the classical splitting decomposition.

When (s_j) converges, the fixed point of iteration (5.1) is the solution of the SSOR preconditioned system $(I - B_\omega)x = c_\omega$.

The stopping criterion was $\|(I - B_\omega)x_k - c_\omega\| < 10^{-8}$ for this linear problem.

We let $n = 70$ and choose $p_1 = 1, p_2 = 1$ and $p_3 = 10$.

For this experiment, the system has dimension 4900×4900 . The width of extrapolation is $m = 20$ and $\omega = 0.5$.

In Table 2, we give the l_2 -norm of the residuals obtained at the end of each cycle and the CPU time for the five methods (MMPE, MPE, RRE, VEA and TEA).

A maximum of 30 cycles was allowed to all the algorithms. Remark that for this experiment, TEA failed to converge and for the VEA we obtained only a residual norm of $9 \cdot 10^{-4}$.

5.2. Example 2

We consider now the following nonlinear partial differential equation:

$$-u_{xx}(x, y) - u_{yy}(x, y) + 2p_1u_x(x, y) + 2p_2u_y(x, y) - p_3u(x, y) + 5e^{u(x,y)} = \phi(x, y) \quad \text{on } \Omega,$$

$$u(x, y) = 1 + xy \quad \text{on } \partial\Omega,$$

Table 3

Method	MMPE	MPE	RRE	VEA	TEA
Number of restarts	20	18	19	22	30
Residual norms	2.9d-09	9.2d-08	2.8d-08	9.6d-09	2.9d-05
CPU time	13.59	13.90	14.72	51.24	65.90

over the unit square of \mathbb{R}^2 with Dirichlet boundary condition. This problem is discretized by a standard five-point central difference formula with uniform grid of size $h = 1/(n + 1)$. We get the following nonlinear system of dimension $N \times N$, where $N = n^2$:

$$AX + 5e^X - b = 0. \quad (5.4)$$

The right-hand-side function $\phi(x, y)$ was chosen so that the true solution is $u(x, y) = 1 + xy$ in Ω .

The sequence (s_j) is generated by using the nonlinear SSOR method. Hence we have $s_{j+1} = G(s_j)$, where

$$G(X) = B_\omega X + \omega(2 - \omega)(D - \omega U)^{-1}D(D - \omega L)^{-1}(b - 5e^X),$$

the matrix B_ω is given in (5.3).

In the following tests, we compare the five extrapolation methods using the SSOR preconditioning. The stopping criterion was $\|x_k - G(x_k)\| < 10^{-8}$.

In our tests, we choose $n = 72$ and hence the system has dimension $N = 4900$. With $m = 20$ and $\omega = 0.5$, we obtain the results of Table 3.

The convergence of the five extrapolation methods above is relatively sensitive to the choice of the parameter ω . We note that for this experiment, the TEA algorithm stagnates after 30 restarts. The VEA algorithm requires more CPU time as compared to the three polynomial extrapolation methods.

6. Conclusion

We have proposed a review of the most known vector extrapolation methods namely the polynomial ones (MMPE, RRE and MPE) and the ε -algorithms (TEA and VEA). We also give some numerical comparison of these methods. The numerical tests presented in this paper show the advantage of the vector polynomial methods. We note also that VEA is numerically more stable than TEA. However, the last two algorithms require more storage and operation counts as compared to the polynomial methods. The advantage of vector extrapolation methods when compared to the classical Krylov subspace methods is that they generalize in a straightforward manner from linear to nonlinear problems.

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Multivariate Hermite interpolation by algebraic polynomials: A survey

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Abstract

This is a survey of that theory of multivariate Lagrange and Hermite interpolation by algebraic polynomials, which has been developed in the past 20 years. Its purpose is not to be encyclopedic, but to present the basic concepts and techniques which have been developed in that period of time and to illustrate them with examples. It takes “classical” Hermite interpolation as a starting point, but then successively broadens the assumptions so that, finally, interpolation of arbitrary functionals and the theory of singularities from algebraic geometry is discussed. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Multivariate Hermite interpolation; Algebraic polynomials; Lagrange; Least interpolation; Lifting schemes

1. Introduction

1.1. Motivation

This is a survey of interpolation by multivariate algebraic polynomials covering roughly the last 20 years.

Why should one study multivariate polynomials? Firstly of all, they are a building block of surprisingly many numerical methods, most often locally. For example, finite elements and splines, both univariate and multivariate, are piecewise polynomials. Secondly, theorems on the quality of approximation of functions or on the quality of a numerical scheme almost invariably reduce to local interpolation by polynomials, even when the approximating functions, respectively the basis of the numerical scheme is of another type. Take any modern textbook on numerical analysis. Except for the part on linear algebra, polynomials are probably mentioned on every third or fourth page. Finally, despite their fundamental importance for numerical methods, the theory of multivariate polynomial

interpolation is underdeveloped and there is hardly any awareness of the issues involved. Indeed, there is hardly any awareness that basic questions are still unresolved.

The three reasons just given to motivate the study of polynomial interpolation are practically oriented. But there is another reason to study polynomials: they are beautiful! Why is number theory so appealing? Because it is beautiful. The objects studied, integers, are the simplest in all of mathematics. I see polynomials as the next step up in the scale of complexity. They are also simple and, again, they are beautiful!

This survey neither intends to be encyclopedic in that all of the newest results are mentioned nor does it intend to be historic, in that it reports on the first occurrence of any particular idea. Instead, the main constructions and the basic ideas behind them will be presented. In addition, many examples will be given. It is my hope that the reader will then *understand* what has been done and be in a position to apply the methods. No proofs will be given, but often the ideas behind the proofs. In addition, the references are mainly chosen according to how well they explain an idea or survey a group of ideas and as to how useful their list of references is.

Most of the results obtained in multivariate interpolation have been obtained in the 30 years surveyed here. The past 10 years have seen a new wave of constructive methods which show how to construct the interpolants and which have been used to find new interpolation schemes. These results are surveyed in detail by Gasca and Sauer in [15], which is also a survey of multivariate interpolation in the same time period. For this reason, these techniques will not be discussed in very much detail here. Rather links to [15] will be made wherever appropriate.

1.2. Interpolation

What is interpolation? In the most general case we will be considering here, we are given a normed linear space Y , a finite linear subspace V of Y , a finite set of bounded functionals $\mathcal{F} = \{F_q\}_{q=1}^m$ and real numbers $\{c_q\}_{q=1}^m$. The *interpolation problem* is to find a $P \in V$ such that

$$F_q P = c_q, \quad q = 1, \dots, m. \quad (1)$$

We will often abbreviate this formulation by saying that we interpolate the functionals \mathcal{F} from V . The interpolating element is called the *interpolant*.

The interpolation problem is called *regular* if the above equation has a unique solution for each choice of values $\{c_q\}_{q=1}^m$. Otherwise, the interpolation is *singular*. In order that an interpolation be regular, it is necessary that

$$\dim V = m = \text{the number of functionals.} \quad (2)$$

Often the values are given by applying the functionals to an element f of Y :

$$c_q = F_q f, \quad q = 1, \dots, m. \quad (3)$$

If so, the interpolation problem can be formulated in a somewhat different way, which we will have cause to use later. Let $\mathcal{G} = \text{span}\{F_q\}_{q=1}^m$. Then \mathcal{G} is an m -dimensional subspace of Y^* , the dual of Y . The interpolation problem (3) is equivalent to: given $f \in Y$, find a $P \in V$ such that

$$FP = Ff \quad \text{for any } F \in \mathcal{G}. \quad (4)$$

An example of all of the above is what I call “classical” Hermite interpolation. To describe it, we first need some polynomial spaces:

$$\Pi_n^d = \left\{ \sum_{|j| \leq n} a_j z^j \mid j \in \mathbb{N}_0^d, z \in \mathbb{R}^d, a_j \in \mathbb{R} \right\}. \tag{5}$$

Here and in the following, we use multivariate notation: $z = (x_1, \dots, x_d)$, $j = (j_1, \dots, j_d)$, $z^j = x_1^{j_1} x_2^{j_2} \cdots x_d^{j_d}$ for $z \in \mathbb{R}^d$ and $j \in \mathbb{N}_0^d$. Moreover $|j| = j_1 + \cdots + j_d$. The above space is called the space of polynomials of *total degree* n and will be our interpolation space V .

The functionals we interpolate are partial derivatives: given a set of distinct points $\{z_q\}_{q=1}^m$ in \mathbb{R}^d and nonnegative integers k_1, \dots, k_m , our functionals are

$$F_{q,\alpha} f = D^\alpha f(z_q), \quad 0 \leq |\alpha| \leq k_q, 1 \leq q \leq m, \tag{6}$$

where

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}.$$

Since

$$\dim \Pi_n^d = \binom{d+n}{d}$$

and the number of partial derivatives (including the function value) to be interpolated at z_q is

$$\binom{d+k_q}{d},$$

we also require that

$$\binom{d+n}{d} = \sum_{q=1}^m \binom{d+k_q}{d}. \tag{7}$$

“Classical” Hermite interpolation, or *Hermite interpolation of total degree* is thus the problem of finding a $P \in \Pi_n^d$ satisfying

$$D^\alpha P(z_q) = c_{q,\alpha}, \quad 0 \leq |\alpha| \leq k_q, 1 \leq q \leq m, \tag{8}$$

for some given values c_q . If all the $k_q = 0$, then we have *Lagrange* interpolation: find $P \in \Pi_n^d$ such that

$$P(z_q) = c_q, \quad 1 \leq q \leq m. \tag{9}$$

Here, of course, $m = \dim \Pi_n^d$.

What determines which kind of multivariate interpolation is the “right” or “most natural” one? The simplest answer is to just look at the univariate case and find the most natural generalization. That is how one arrives at the multivariate interpolation just described. But, as we shall see, there are other perfectly good multivariate interpolations. For, while in the univariate case, the polynomial interpolation space, namely Π_n^1 , is canonical, in the multivariate case, we have many polynomial spaces of the same dimension. The derivatives we have chosen are in the direction of the coordinate axes. See Section 3 for Hermite interpolations involving directional derivatives. Moreover, we will

see (in Section 4) that interpolating not point values of functions or their derivatives, but mean values of them over line segments, triangles, etc., leads to interpolation schemes retaining many of the properties of univariate interpolation.

Other criteria for the choice of the interpolation derive from the use to which the interpolant is to be put. If, for example, the interpolant interpolates the values resulting from the application of the functionals to a function, as in (3), then one would like to know how well the interpolant approximates the function (in the norm of Y). and tailor the interpolation accordingly. For exactly this reason, there is a host of papers concerned with developing Newton like interpolations. Since this aspect of polynomial interpolation will not be emphasized here, the reader can find them in the survey paper by Gasca and Sauer [15], and in the papers by Sauer and Xu [37,38].

Often such interpolations allow more precise statements about the error of approximation. In addition, these methods are numerically quite stable.

For finite elements, other properties play an important role. Two of them are that the dimension of interpolation space, V , be as small as possible to attain the desired global continuity and that the interpolation spaces be affinely invariant. Consequently, V may not be a full space Π_n^d for some n, d , but may lie between two such spaces $\Pi_n^d \subsetneq V \subsetneq \Pi_{n+1}^d$. Many examples of such interpolations can be found in [7].

As a last application which would require special properties from the interpolant, let me mention cubature formulas. As in the univariate case, one method for constructing cubature formulas is to base them on Lagrange interpolation at the zeros of orthogonal polynomials. Here the nodes are prescribed and a polynomial space must be constructed so that interpolation at these nodes is regular. Again, these spaces will, in general, not coincide with a Π_n^d .

Of course, many nonpolynomial multivariate interpolation methods have been developed. See [40] for a survey on scattered data interpolation.

2. The issues involved

2.1. Univariate interpolation

Let us first look at univariate interpolation, since everything works well there. Given m distinct points $\{z_q\}_{q=1}^m$ in \mathbb{R}^1 and m real values $\{c_q\}_{q=1}^m$, there is one and only one polynomial $P \in \Pi_{m-1}^1$ with

$$P(z_q) = c_q, \quad q = 1, \dots, m, \tag{10}$$

i.e., the univariate Lagrange interpolation problem is regular for any set of nodes. The same is true of univariate Hermite interpolation: Given a nodal set $Z = \{z_q\}_{q=1}^m$, integers k_q and values $c_{q,\alpha}$ for $0 \leq \alpha \leq k_q$ and $q = 1, \dots, m$, there is one and only one polynomial $P \in \Pi_n^1$, where

$$n = \sum_{q=1}^m (k_q + 1) - 1, \tag{11}$$

such that

$$D^\alpha P(z_q) = c_{q,\alpha} \quad 0 \leq \alpha \leq k_q, \quad q = 1, \dots, m, \tag{12}$$

i.e., the univariate Hermite interpolation problem is regular for any nodal set and for any choice of derivatives to be interpolated. A word of caution here. There is another type of univariate in-

terpolation, called Birkhoff interpolation, which interpolates derivatives but differs from Hermite interpolation in that gaps in the derivatives are allowed. In this theory, for example, one could interpolate $f(z_q)$ and $f''(z_q)$ but not $f'(z_q)$. Such interpolations are not necessarily regular. See [27] for the univariate theory and [28] for the multivariate theory of Birkhoff interpolation.

How does one prove regularity? There are several ways. One method is constructive in that one finds a basis $\lambda_q, q = 1, \dots, m$ of Π_n^1 (or of V in general) dual to the functionals we are interpolating in the sense that $F_q \lambda_r = \delta_{qr}$. The elements of such a basis are sometimes called the *fundamental functions* of the interpolation. The Lagrange interpolant, for example, could then be written as

$$P(z) = \sum_{q=1}^m f(z_q) \lambda_q(z), \tag{13}$$

if the data to be interpolated are given by $c_q = f(z_q)$. The fundamental functions then satisfy $\lambda_r(z_q) = \delta_{qr}$. For Lagrange interpolation, it is easy to find the dual basis

$$\lambda_q(z) = \frac{\prod_{1 \leq r \leq m, r \neq q} (z - z_r)}{\prod_{1 \leq r \leq m, r \neq q} (z_q - z_r)}. \tag{14}$$

It is also not hard to find the dual basis for univariate Hermite interpolation.

Another, but nonconstructive approach to proving regularity starts by choosing a basis for Π_n^1 (or of V in general). Then Eq. (10) or (12) (or (1) in general) become a linear system of equations for the coefficients of the representation of the interpolant in the chosen basis. We will call the matrix M of this linear system the *Vandermonde matrix* and the determinant D of M the *Vandermonde determinant*. We sometimes write $M(F, V)$ or $M(Z)$ to make the dependency of M or D on the functionals and on the details of the interpolation more explicit.

The method is based on the fact that our interpolation is regular if and only if $D \neq 0$. The interpolation is singular if $D = 0$. For Lagrange interpolation, we have the famous formula for the (original) Vandermonde determinant

$$D(Z) = \prod_{1 \leq q < r \leq m} (z_q - z_r)$$

if the monomial basis $\{x^z\}_{z=1}^m$ is taken for Π_{m-1}^1 . We can immediately read off of this formula that Lagrange interpolation is regular if and only if the nodes z_q are distinct. A similar formula can be found for the Vandermonde determinant of Hermite interpolation.

A third method, another constructive method, is known as the Newton method. The idea is to start by interpolating one functional, then increase the number of functionals interpolated stepwise (either one at a time, or in packets) until the required set of functionals is interpolated. At each step, one adds a polynomial to the previous interpolant, which interpolates zero values for the functionals already interpolated. In this way, the work done in the previous steps is not spoiled.

Let us carry this out for Lagrange interpolation of the function values c_q at the nodes $z_q, q = 1, \dots, m$. We take $P_1(z) \equiv c_1$. Then P_1 interpolates the first functional (functional evaluation at z_1) and $P_1 \in \Pi_0^1$. Let $Q_2(z) = z - z_1$. Then $Q_2(z_1) = 0$ and $R_2(z) = c_2 Q_2(z) / Q_2(z_2)$ vanishes at z_1 and takes the value c_2 at z_2 . So $P_2 = P_1 + R_2$ interpolates the first two functionals. After finding a

polynomial $P_j \in \Pi_{j-1}^1$ which interpolates the first j values, We take

$$Q_{j+1}(z) = \prod_{q=1}^j (z - z_q).$$

Then $R_{j+1}(z) = c_{j+1}Q_{j+1}(z)/Q_{j+1}(z_{j+1})$ vanishes at the first j nodes while taking the value c_{j+1} at z_{j+1} . Let $P_{j+1} = P_j + R_{j+1}$. Then $P_{j+1} \in \Pi_j^1$ interpolates the first $j + 1$ values.

The formula for the Newton interpolant to a continuous function f is

$$P(f)(x) = \sum_{q=1}^m f[z_1, \dots, z_q] \prod_{r=1}^{q-1} (x - z_r), \tag{15}$$

where the divided difference $f[z_r, \dots, z_q]$, $r \leq q$, is defined by

$$f[z_r] = f(x_r), \tag{16}$$

$$f[z_r, \dots, z_q] = \frac{f[z_r, \dots, z_{q-1}] - f[z_{r+1}, \dots, z_q]}{z_r - z_q}. \tag{17}$$

The Newton form of the interpolant is particularly suitable for obtaining error estimates.

We have gone through these well-known univariate methods in such detail because, as we will see, many multivariate proofs and constructions are based on these principles, although the details may be much more involved.

2.2. Multivariate Lagrange interpolation

I claim that univariate and multivariate Lagrange interpolation are two very different animals. To see what I mean, let us look at the first nontrivial bivariate Lagrange interpolation: the interpolation of two values at two nodes z_1, z_2 in \mathbb{R}^2 . But which space of polynomials should we use? The space of linear polynomials Π_1^2 is spanned by 1, x and y and thus has dimension 3, while the space of constants, Π_0^2 , has dimension only one! Our interpolation falls into the gap. There is no “natural” space of polynomials which fits our problem, or at least no obvious natural space.

Now let us try Lagrange interpolation on three nodes $Z = \{z_1, z_2, z_3\}$. We choose $V = \Pi_1^2$, so that (2) is satisfied. Choosing the monomial basis for Π_1^2 , the Vandermonde determinant of the interpolation is

$$D(Z) = (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1),$$

where $z_q = (x_q, y_q)$. If the three nodes are the vertices of a non-degenerate triangle, then $D(Z) \neq 0$. But if the nodes are collinear, say $z_1 = (0, 0)$, $z_2 = (1, 0)$ and $z_3 = (2, 0)$, one can check that $D(Z)$ vanishes and the interpolation is singular.

Thus, we have seen two differences between univariate and multivariate Lagrange interpolation. In the multivariate case, it is not clear which interpolation spaces we should choose and, even when there is an easy choice, the interpolation is regular for some knot sets and singular for others. We can be more precise about the latter statement.

Theorem 1. *Let $Z = \{z_q\}_{q=1}^m \subset \mathbb{R}^d$ and $n \in \mathbb{Z}_0$ such that $m = \dim \Pi_n^d$. Then Lagrange interpolation is regular for almost all choices of Z in the Lebesgue measure of \mathbb{R}^{md} .*

In fact, the Vandermonde determinant $D(Z)$ of the system of equations for the coefficients of the interpolant is a polynomial in the coordinates of the nodes and therefore either vanishes identically or is nonzero almost everywhere.

The most general statement one can make about Z for which Lagrange interpolation is regular is that Z does not lie on an algebraic curve of degree not exceeding n . However, this statement is almost a tautology and is not constructive.

Many people have worked on finding explicit formulas for arrays for which Lagrange interpolation is regular. Some of them are quite ingenious and beautiful, but all of them are only *necessary* conditions for regularity. We will see some of them in Section 5.

2.3. Multivariate Hermite interpolation

Everything we have said about Lagrange interpolation also holds for multivariate Hermite interpolation including Theorem 1. However, yet another complication rears its head. Consider the simplest non-trivial bivariate Hermite interpolation. This is interpolating function values and both first derivatives at each of two nodes z_1 and z_2 in \mathbb{R}^2 . We interpolate using quadratic polynomials, i.e., polynomials from Π_2^2 . Note that the condition (2) is satisfied. There are 6 functionals to be interpolated and $\dim \Pi_2^2 = 6$. We will show that this interpolation is *singular* for *all* choices of nodes z_1, z_2 . We will be seeing this example quite often. For this reason, I call it *my favorite singular Hermite interpolation*.

A common method used to demonstrate the singularity of this interpolation is based on the observation that an interpolation satisfying the condition (2) is singular if and only if there is a nonzero polynomial which satisfies the homogeneous interpolation conditions. That is, there is a $P \in V$ satisfying (9) with all $c_q = 0$.

Now returning to our Hermite interpolation, let $\ell(z) = 0$ be the equation of the straight line joining z_1 and z_2 . ℓ is a linear polynomial, i.e., in Π_1^1 . So $\ell^2 \in \Pi_2^2$. We see that ℓ^2 and both of its first derivatives vanish at both z_1 and z_2 . Thus the interpolation is singular.

Sitting back and sifting through the rubble, we are forced to distinguish between three possibilities:

- (a) the interpolation is regular for any choice of node set,
- (b) the interpolation is regular for almost any choice of node set, but not for all,
- (c) the interpolation is singular for any choice of node set.

In the situation where the functionals to be interpolated depends on the choice of the nodes, as for Lagrange or Hermite interpolation, we will say that the interpolation is *regular* if (a) holds, that it is *a.e. regular* if (b) holds, and that it is *singular* if (c) holds.

We have just shown that both (b) and (c) occur. What about (a)? In the next section, we will show that for Hermite interpolation, (a) can occur if and only if the interpolation is on one node ($m = 1$). This is called *Taylor* interpolation. In that section we also run through the known cases of almost everywhere regular and of singular Hermite interpolations.

In Section 4, we will look at two alternatives to “classical” Hermite interpolation. The first one “lifts” univariate Hermite interpolation to higher dimensions. The second, called the “least interpolation”, constructs the polynomial space to match the functionals and can be used in a much more general context.

The above proof of singularity brings us quite close to a classical question of algebraic geometry.

Given the functionals (6) of Hermite interpolation, what is the lowest degree of a nonzero polynomial Q satisfying the homogeneous equation? One then says that Q has singularities of order $k_q + 1$ at z_q . If (7) is satisfied, then the interpolation is singular if and only the lowest degree is the n of (7). But one can still formulate the question even if (7) does not hold. This question is considered in Section 6.

3. Multivariate Hermite interpolation

3.1. Types of Hermite interpolation

Although we only discussed classical Hermite interpolation in the introduction, a type which we will denote by *total degree* from now on, there are other types. They can be subsumed in the following definition of Hermite interpolation from [38], which replaces derivatives in the coordinate directions by directional derivatives.

Let $z \in \mathbb{R}^d$ and $m \in \mathbb{N}_0$. Given an index set

$$E = (1 | \varepsilon_1^1, \dots, \varepsilon_{r_1}^1 | \dots | \varepsilon_1^m, \dots, \varepsilon_{r_m}^m), \tag{18}$$

where $\varepsilon_i^k = 1$ or 0 , and a diagram $T_z = T_{z,E}$ defined by

$$T_z = (z | y_1^1, \dots, y_{r_1}^1 | \dots | y_1^m, \dots, y_{r_m}^m), \tag{19}$$

where $y_i^k \in \mathbb{R}^d$ and $y_i^k = 0$ if $\varepsilon_i^k = 0$, one says that E is of tree structure if for each $\varepsilon_i^k = 1$, $k > 1$, there exists a unique $j = j(i)$ such that $\varepsilon_j^{k-1} = 1$. ε_j^{k-1} is called the predecessor of ε_i^k . Moreover, the edges of the tree connect only at a vertex and its predecessor. Note that this definition of a tree is more restrictive than the usual definition of a tree in graph theory.

The trees used here will be specified by their maximal chains. A sequence $\mu = (i_1, \dots, i_k)$ is called a chain in the tree structure E , if $\varepsilon_{i_1}^1 = \dots = \varepsilon_{i_k}^k = 1$, where for each j , $1 \leq j \leq k-1$, $\varepsilon_{i_j}^k$ is the predecessor of $\varepsilon_{i_{j+1}}^{k+1}$. It is called a maximal chain if its last vertex $\varepsilon_{i_k}^k$ is not the predecessor of another element in E .

Let μ be a chain of T_z , ($\mu \in T_z$). Define

$$y^\mu = y_{i_1}^1 \cdots y_{i_k}^k; \quad \sigma(\mu) = k \tag{20}$$

and the differential operator

$$D_{y^\mu}^{\sigma(\mu)} = D_{y_{i_1}^1} \cdots D_{y_{i_k}^k}. \tag{21}$$

The chain and the diagram T_z define a product of directional derivatives.

To define Hermite interpolation at a point z , we choose a tree T_z with the additional property that every vertex of T_z is connected to the root z by exactly one chain. Then Hermite interpolation at the point z is defined to be the interpolation of all of the functionals

$$D_{y_{i_1}^1} \cdots D_{y_{i_k}^k} f(z) \tag{22}$$

associated to the vertices of the tree via the unique chain connecting that vertex to the root. One of the important characteristics of this definition is that there are no gaps in the chains of increasing orders of derivatives. Hermite interpolation at nodes z_1, \dots, z_m would be interpolating the functionals

of Eq. (22) for trees T_{z_1}, \dots, T_{z_m} by polynomials from Π_n^d . It is assumed that the number of functionals interpolated equals the dimension of the interpolating space.

By restricting the directions y_j^k to the coordinate directions and choosing the tree appropriately, one may obtain Hermite interpolation of total degree.

Another special case is denoted by *Hermite interpolation of coordinate degree*. To motivate this second type, let us look at Lagrange interpolation on a node set which forms a rectangular grid in \mathbb{R}^2 . Let $x_1 < x_2 < \dots < x_{n_1+1}$ and $y_1 < y_2 < \dots < y_{n_2+1}$ be points in \mathbb{R} . It seems natural to measure the values of a function on the rectangular grid

$$Z = \{(x_i, y_j) \mid 1 \leq i \leq n_1 + 1; 1 \leq j \leq n_2 + 1\}. \tag{23}$$

Now let us interpolate these values. Which space of polynomials fits this grid? Surely not some Π_n^2 ! Instead, we introduce the space of polynomials $\Pi_{(n_1, \dots, n_d)}^d$ of *coordinate degree* (n_1, \dots, n_d) .

It is convenient to first introduce more general polynomial spaces of which the space of polynomials of total degree will be a special case. Let $A \subset \mathbb{N}_0^d$. Then the polynomial space Π_A is defined by

$$\Pi_A = \left\{ \sum_{j \in A} a_j z^j \right\}. \tag{24}$$

For example, we recover the space Π_n^d in the form $\Pi_n^d = \Pi_A$ with

$$A = \{j \in \mathbb{N}_0^d \mid |j| \leq n\}.$$

Now the space of polynomials $\Pi_{(n_1, \dots, n_d)}^d$ of *coordinate degree* (n_1, \dots, n_d) is Π_A with

$$A = \{j \in \mathbb{N}_0^d \mid 0 \leq j_i \leq n_i, i = 1, \dots, d\}. \tag{25}$$

For Lagrange interpolation on the grid (23), at least, $\Pi_{(n_1, \dots, n_d)}^d$ is the right space. Lagrange interpolation on the grid (23) with polynomials from $\Pi_{(n_1, \dots, n_d)}^d$ is regular.

This motivates the definition of *Hermite interpolation of coordinate degree*: Let a positive integer m , d -tuples of non-negative integers (n_1, \dots, n_d) , $k_q = (k_{q,1}, \dots, k_{q,d})$ for $q = 1, \dots, m$, a node set $Z = \{z_1, \dots, z_m\}$, $z_q \in \mathbb{R}^d$ and a set of values $c_{q,\alpha}$ be given. Find a $P \in \Pi_{(n_1, \dots, n_d)}^d$ with

$$D^\alpha P(z_q) = c_{q,\alpha} \quad 0 \leq \alpha_i \leq k_{q,i}, \quad 1 \leq i \leq d, \quad 1 \leq q \leq m. \tag{26}$$

The numbers n and k_q are assumed to satisfy

$$\prod_{i=1}^d (n_i + 1) = \sum_{q=1}^m \prod_{i=1}^d (k_{q,i} + 1). \tag{27}$$

If we interpolate the same derivatives at each node, then we have *uniform* Hermite interpolation of type either total or coordinate degree. Of course, (7) and (27) are to be satisfied with all k_q equal.

3.2. Everywhere regular schemes

In this subsection, we will consider those interpolation schemes which are regular for any location of the nodes. For Hermite interpolation of type either total or coordinate degree, this is only the case if there is only one node in the interpolation, $Z = \{z\}$. Such interpolations are called Taylor

interpolations. Then there is a one-to-one correspondence between the partial derivatives to be interpolated (at z) and the monomial basis of Π_n^d , respectively $\Pi_{(n_1, \dots, n_d)}^d: D^z \leftrightarrow z^z$. The Vandermonde matrix based on the monomial basis of the polynomial space, say in the lexicographical ordering, with the derivatives taken in the same order is an upper triangular matrix with the non-zero diagonal entries $\alpha!$. So the determinant never vanishes. We have proved that Taylor interpolation is regular for any choice of the node.

It is, in fact, the only such multivariate Hermite interpolation, see [28].

Theorem 2. *In \mathbb{R}^d , $d \geq 2$, the only Hermite interpolation of type total or coordinate degree, which is regular for all choices of the nodes, is Taylor interpolation.*

This theorem is also true for more general polynomial spaces. The most general form I know is by Jia and Sharma, [24]. To formulate it, we need some terminology. Let $V \subset \Pi^d$ be a finite-dimensional space of polynomials. V is said to be scale invariant if $P(az) \in V$ for any $a \in \mathbb{R}$ and any $P \in V$. Also, for any polynomial $P = \sum_j a_j z^j$, the differential operator $P(D)$ is defined by

$$P(D)f = \sum_j a_j D^j f. \tag{28}$$

Now let Z be a node set. To each $z_q \in Z$, let there be associated a finite-dimensional space of polynomials $V_q \subset \Pi^d$. We choose any bases $P_{q,1}, \dots, P_{q,r(q)}$ of V_q , $q = 1, \dots, m$ (then $r(q) = \dim V_q$), values $c_{q,i}$ and a set $A \in \mathbb{N}_0^d$. The *Abel-Goncharov* interpolation problem is to find a polynomial $Q \in \Pi_A$ (recall definition (24)) satisfying

$$P_{q,i}(D)Q(z_q) = c_{q,i}, \quad 1 \leq i \leq r(q), \quad q = 1, \dots, m. \tag{29}$$

The choice of the bases does not affect the regularity of the interpolation.

Theorem 3. *Using the above notation, let $V, V_q, q = 1, \dots, m$, be scale invariant. Then Abel-Goncharov interpolation (29) is regular for any node set if*

$$V = \bigoplus_{q=1}^m V_q. \tag{30}$$

For a special case, Jia and Sharma prove more

Theorem 4. *Let $A \subset \mathbb{N}_0^d$. Let $A_q \subset A, q = 1, \dots, m, V = \Pi_A, V_q = \Pi_{A_q}, q = 1, \dots, m$. Then Abel-Goncharov interpolation (29) is regular for any node set Z if and only if A is the disjoint sum of the $A_q, q = 1, \dots, m$.*

This theorem implies Theorem 2. For example, for Hermite interpolation of type total degree, $\Pi_n^d = \Pi_A$ with $A = \{j \mid j \in \mathbb{N}_0^d, |j| \leq n\}$ while the derivatives to be interpolated derive from the polynomial spaces $V_q = \Pi_{A_q}$ with $A_q = \{j \mid j \in \mathbb{N}_0^d, |j| \leq k_q\}$. The same holds for Hermite interpolation of type coordinate degree. It also includes a similar theorem for multivariate Birkhoff interpolation.

In view of the these results, Jia and Sharma formulated the conjecture

Conjecture 5. Let V and $\{V_q\}_{q=1}^m$ be scale-invariant subspaces of Π^d such that

$$\bigcup_{q=1}^m V_q \subset V.$$

Then Abel-Goncharov interpolation (29) is regular if and only if (30) holds.

3.3. A.e. regular Hermite interpolation of type total degree in \mathbb{R}^2

From the previous section, we have seen that multivariate Hermite interpolation can, except for some very special cases, be at most regular for almost all choices of nodes. We denote this as being regular a.e. Not too much is known about even a.e. regular Hermite interpolation of type total degree. Gevorkian et al. [16] have proven

Theorem 6. Bivariate Hermite interpolation of type total degree (8) is regular a.e. if there are at most 9 nodes with $k_q \geq 1$.

Sauer and Xu [38] have proven

Theorem 7. Multivariate Hermite interpolation of type total degree (8) in \mathbb{R}^d with at most $d + 1$ nodes having $k_q \geq 1$ is regular a.e. if and only if

$$k_q + k_r < n$$

for $1 \leq q, r \leq m, q \neq r$.

The authors of Theorem 6 have also considered Hermite interpolation of type total degree from the point of view of algebraic geometry. These results will be discussed in Section 6. A conjecture due to them and Paskov [18,34], simultaneously does fit in here. Let us use the stenographic notation $\mathcal{N} = \{n; s_1, \dots, s_m\}$ to stand for Hermite interpolation of type total degree on m nodes interpolating derivatives of order up to $k_q = s_q - 1$ at z_q by bivariate polynomials of degree n . We are using the standard notation of algebraic geometry here, working with orders of singularities s_q . Also, we will not be much concerned about the node set Z , since we are only interested in regularity a.e. In addition, we allow an s_q to be 0. This just means that there is no interpolation condition at that node. We also do not demand that the condition (7) requiring that the number of degrees of freedom in the interpolation space equals the number of functionals to be interpolated, holds.

With this freedom, we do not have interpolations in the strict sense of Equation 2 any more, so let us just call them *singularity schemes*. We introduce addition among singularity schemes just by vector addition. If $\mathcal{N} = \{n; s_1, \dots, s_m\}$ and $\mathcal{R} = \{r; t_1, \dots, t_m\}$, then

$$\mathcal{N} + \mathcal{R} = \{n + r; s_1 + t_1, \dots, s_m + t_1\}. \tag{31}$$

We can add singularity schemes of different lengths by introducing zeros in the shorter of them.

The relevance of this addition is that if $Q_1 \in \Pi_n^2$ satisfies the homogeneous interpolation conditions of \mathcal{N} and if $Q_2 \in \Pi_r^2$ satisfies the homogeneous interpolation conditions of \mathcal{R} , where \mathcal{N} and \mathcal{R} are of the same length and refer to the same nodes, then $Q_1 Q_2 \in \Pi_{n+r}^2$ satisfies the homogeneous interpolation conditions of $\mathcal{N} + \mathcal{R}$,

The conjecture is

Conjecture 8. *Let \mathcal{N} correspond to a Hermite interpolation of type total degree (that is condition (7) holds). Then \mathcal{N} is singular if and only if there are schemes $\mathcal{R}_i = \{r_i; t_{i,1}, \dots, t_{i,m}\}, i = 1, \dots, p$ satisfying*

$$\binom{r_i + 2}{2} > \sum_{q=1}^m \binom{t_{i,q} + 2}{2}, \quad i = 1, \dots, p,$$

such that

$$\mathcal{N} = \sum_{i=1}^p \mathcal{M}_i.$$

The sufficiency part of this theorem is easy to see. There are always nonzero polynomials Q_i satisfying the homogeneous interpolation conditions of $\mathcal{R}_i, i = 1, \dots, p$, since each of them can be found by solving a linear system of homogeneous equations with less equations than unknowns. By the above remark, $\prod_{i=1}^p Q_i \in \Pi_n^2$ is a nonzero polynomial satisfying the homogeneous conditions for \mathcal{N} .

We have already seen an example of this. It is our favorite singular Hermite interpolation: the interpolation of first derivatives at two nodes in \mathbb{R}^2 by polynomials from Π_2^2 . In the notation used here, this is the singularity scheme $\mathcal{N} = \{2; 2, 2\}$. It can be decomposed as $\mathcal{N} = \mathcal{R} + \mathcal{S}$, with $\mathcal{R} = \mathcal{S} = \{1; 1, 1\}$. More singular Hermite interpolations constructed using this idea can be found in [34; 28 Chapter 4].

There are essentially no other results for the a.e. regularity of general Hermite interpolation of total degree. More is known for uniform Hermite interpolation of total degree. The results which follow can be found in [38,28].

The simplest case of uniform Hermite interpolation is, of course, Lagrange interpolation in which partial derivatives of order zero are interpolated at each node. The number of nodes in $\dim \Pi_n^2$ for some n and it is regular a.e.

The next case is when all partial derivatives up to first order are interpolated at each node. Condition (7) is then

$$\binom{n + 2}{2} = m \binom{1 + 2}{2} = 3m. \tag{32}$$

This equation has a solution for n and m if and only if $n = 1, 2 \pmod 3$.

Theorem 9. *For all n with $n = 1, 2 \pmod 3$, bivariate uniform Hermite interpolation of type total degree interpolating partial derivatives of order up to one is regular a.e., except for the two cases with $n = 2$ (then $m = 2$) and $n = 4$ (then $m = 5$). The two exceptional cases are singular.*

Note that our favorite singular Hermite interpolation is included. The smallest non-Taylor a.e. regular case is for $n = 5$. The interpolation is then on 7 nodes.

The method of the proof of this and the following two theorems is to show that the Vandermonde determinant does not vanish identically by showing that one of its partial derivatives is a nonzero constant. The technique used to show this is the “coalescence” of nodes and, roughly speaking, tries to reduce the number of nodes of the interpolation until a Taylor interpolation is obtained.

If all partial derivatives up to second order are interpolated at each node, condition (7) becomes

$$\binom{n+2}{2} = m \binom{2+2}{2} = 6m. \quad (33)$$

This equation has a solution for n and m if and only if $n = 2, 7, 10, 11 \pmod{12}$.

Theorem 10. *For all n with $n = 2, 7, 10, 11 \pmod{12}$, bivariate uniform Hermite interpolation of type total degree interpolating partial derivatives of order up to two is regular a.e.*

The smallest non-Taylor a.e. regular case is for $n = 7$. The interpolation is then on 12 nodes.

For third derivatives, we must have $n = 3, 14, 18, 19 \pmod{20}$.

Theorem 11. *For all n with $n = 3, 14, 18, 19 \pmod{20}$, bivariate uniform Hermite interpolation of type total degree interpolating partial derivatives of order up to three is regular a.e.*

The smallest non-Taylor a.e. regular case is for $n = 14$. The interpolation is then also on 12 nodes.

For related results from algebraic geometry, see Section 6.

3.4. A.e. regular bivariate Hermite interpolation of type coordinate degree in \mathbb{R}^2

No theorems about the a.e. regularity of general Hermite interpolation of type coordinate degree in \mathbb{R}^d , as defined in (26), are known except for the relatively simple one given at the end of this subsection. But there are a few things known of the uniform case. If we want to interpolate all partial derivatives of order up to k_1 in x and to k_2 in y from $\Pi_{(n_1, n_2)}^2$, then

$$(n_1 + 1)(n_2 + 1) = m(k_1 + 1)(k_2 + 1) \quad (34)$$

must hold. The proofs of the the following theorems, all of which can be found in [28], are based on the same techniques as for the theorems on a.e. regularity of uniform Hermite interpolation of type total degree in the previous subsection.

Theorem 12. *If (34) is satisfied, and either $k_1 + 1$ divides $n_1 + 1$ or $k_2 + 1$ divides $n_2 + 1$, then bivariate uniform Hermite interpolation of type coordinate degree interpolating all partial derivatives of order up to k_1 in x and to k_2 in y from $\Pi_{(n_1, n_2)}^2$ is a.e. regular.*

This is more general than tensor product interpolation, since there one would have that both $k_1 + 1$ divides $n_1 + 1$ and $k_2 + 1$ divides $n_2 + 1$. If $n_1 = n_2 = n$ and $k_1 = k_2 = k$, which is a kind of (uniform)² Hermite interpolation, then (34) forces k to divide n and we have

Corollary 13. *Bivariate uniform Hermite interpolation of type coordinate degree interpolating all partial derivatives of order up to k in x and in y from $\Pi_{(n_1, n_2)}^2$ is a.e. regular.*

This corollary also holds in \mathbb{R}^d , but theorems like Theorem 12 in \mathbb{R}^d require much more restrictive assumptions.

As for uniform Hermite interpolation of type total degree, interpolations involving only lower order derivatives can be taken care of completely.

Theorem 14. *For all combinations, except two, of k_1, k_2 with $0 \leq k_1, k_2 \leq 2$ and n_1, n_2 with $0 \leq k_1 \leq n_1, 0 \leq k_2 \leq n_2$ satisfying (34), uniform bivariate Hermite interpolation of type coordinate degree interpolating all partial derivatives of order up to k_1 in x and to k_2 in y from $\Pi_{(n_1, n_2)}^2$ is a.e. regular. The two exceptional cases are $k_1 = 1$ and $k_2 = 2$ from $\Pi_{(2, 3)}^2$ and the corresponding interpolation with x and y interchanged. These are singular.*

This theorem includes cases Theorem 12 does not cover. For example, interpolating partial derivatives of first order in x and second order in y at each of eight nodes from $\Pi_{(8, 3)}^2$ is regular a.e. But Theorem 12 does not apply since neither 2 divides 9 nor does 3 divide 4.

We conclude this subsection with a theorem on non-uniform interpolation.

Theorem 15. *A bivariate Hermite interpolation of type coordinate degree interpolating all partial derivatives of order up to $k_{q,1}$ in x and to $k_{q,2}$ in y at $z_q, q = 1, \dots, m$ from $\Pi_{(n_1, n_2)}^2$ is a.e. regular if the rectangle $(0, n_1 + 1) \times (n_2 + 1)$ is the disjoint union of the translates of the rectangles $(0, k_{q,1} + 1) \times (k_{q,2} + 1) q = 1, \dots, m$.*

This theorem does not hold in \mathbb{R}^d for $d \geq 3$.

3.5. Singular Hermite interpolations in \mathbb{R}^d

The general trend of the results of this subsection will be that a Hermite interpolation in \mathbb{R}^d will be singular if the number of nodes is small, typically $m \leq d + 1$. Of course, Taylor interpolations are excepted. Also Lagrange interpolation by linear polynomials ($m = d + 1$) is excluded. The theorems can all be found in [28,38].

Theorem 16. *Hermite interpolation of type total degree in $\mathbb{R}^d, d \geq 2$, is singular if the number of nodes satisfies $2 \leq m \leq d + 1$ except for the case of Lagrange interpolation which is a.e. regular.*

Implicitly, condition (7) is assumed to be satisfied.

The theorem includes our favorite singular Hermite interpolation. It is proved showing that the interpolation restricted to a certain hyperplane is not solvable.

One application of this theorem is a negative result related to the construction of finite elements. The statement is that there is no finite element interpolating all derivatives up to a given order (which may depend on the vertex) at each of the vertices of a tetrahedron in $\mathbb{R}^d, d \geq 2$, which interpolates from a complete space, say Π_n^d . The existence of such an element would have been desirable as it would have combined the highest degree approximation, $n + 1$, and global continuity available for a given amount of computational effort.

For interpolation of type coordinate degree, we have

Theorem 17. *Bivariate uniform Hermite interpolation of type coordinate degree interpolating all partial derivatives of order k_1 in x and to k_2 in y at either two or three nodes from $\Pi_{(n_1, n_2)}^2$ is singular unless either $p_1 + 1$ divides $n_1 + 1$ or $p_2 + 1$ divides $n_2 + 1$.*

The exceptional cases are regular by Theorem 12.

Singular uniform Hermite interpolation schemes on more than $d + 1$ nodes in \mathbb{R}^d are hard to find. Here are some for uniform Hermite interpolation of type total degree due to Sauer and Xu [38].

Theorem 18. *Uniform Hermite interpolation of type total degree interpolating all partial derivatives of order up to k at each of m nodes in \mathbb{R}^d by polynomials from Π_n^d is singular if*

$$m < \frac{(n+1) \cdots (n+d)}{((n-1)/2+1) \cdots ((n-1)/2+d)}.$$

In \mathbb{R}^2 , the smallest example is covered by this theorem is the interpolation of all partial derivatives of up to first order at each of 5 nodes by quartic polynomials.

3.6. Conclusions

We have seen that Hermite interpolation of either total or coordinate degree type is regular if $m = 1$, is singular if there are not too many nodes and, for uniform Hermite interpolation of type coordinate degree, there are no other exceptions if we are interpolating derivatives of order up to one, two or three. Really general theorems for a.e. regularity of interpolations with arbitrarily high derivatives are not known. The same holds for the results obtained by the methods of algebraic geometry, as we will see in Section 6.

In this section, we have assiduously ignored one of the essential components of interpolation. Most of the theorems of this section concerned a.e. regularity. To use these interpolations, one must find concrete node sets for which the interpolations are regular. Only for Lagrange interpolation are any systematic results known. Otherwise, nothing is known. For this reason, special constructions of interpolations which include the node sets, such as those in Sections 5 and 6, are of importance, even if the interpolation spaces are not complete spaces Π_n^d .

4. Alternatives to classical multivariate Hermite interpolation

4.1. Lifting schemes

Our extension of univariate to “classical” multivariate Hermite interpolation, namely to multivariate Hermite interpolation of type total degree, has one glaring defect. It is not regular for any choice of nodes. It is in fact possible to get rid of this unfavorable property, but alas, at a price. The method to be introduced here, called “lifting”, yields a multivariate interpolation which is formulated exactly as in the univariate case. In our context, it was introduced by Goodman [19] motivated by the first special cases, those of Kergin [25], Hakopian [21] and of Cavaretta et al. [5]. For a more complete survey, see the book [1] of Bojanov, Hakopian and Sahakian, or the thesis of Waldron [43] and the references therein.

Let us first formulate it for Lagrange interpolation: given m nodes z_1, \dots, z_m in \mathbb{R}^d and values c_1, \dots, c_m , there is a polynomial $P \in \Pi_{m-1}^d$ which interpolates the values

$$P(z_q) = c_q, \quad q = 1, \dots, m. \tag{35}$$

So what is the problem? The problem is that $\dim \Pi_{m-1}^d$ is much larger than m , so that Eq. (35) does not determine P uniquely. As we will see, there are many different ways to add additional interpolation conditions in order to make the interpolant unique.

But wait. Let us be more cautious. If the nodes can be chosen arbitrarily, can we be sure that there is at least one P in Π_{m-1}^d satisfying (35). Severi, [41], has already answered this question for us in the context of Hermite interpolation.

We will say that a Hermite interpolation (of type total degree) is *solvable* with polynomials from Π_n^d if given m , orders $\{k_q\}_{q=1}^m$ and values $c_{q,\alpha}$ for $0 \leq |\alpha| \leq k_q$, $q = 1, \dots, m$, there is, for any node set $Z = \{z_q\}_{q=1}^m$, a $P \in \Pi_n^d$ with

$$D^\alpha P(z_q) = c_{q,\alpha} \quad 0 \leq |\alpha| \leq k_q, q = 1, \dots, m. \tag{36}$$

Theorem 19. *Let m and nonnegative integers $\{k_q\}_{q=1}^m$ be given. A necessary and sufficient condition that Hermite interpolation of type total degree be solvable with polynomials from Π_n^d is that*

$$n + 1 \geq \sum_{q=1}^m (k_q + 1).$$

Thus, we see that Lagrange interpolation on m nodes is solvable from Π_{m-1}^d . Note also that the condition is the same for any dimension d . Actually, the case of Lagrange interpolation can be done directly. One can construct a Lagrange interpolating function from Π_{m-1}^d for a node by taking the product of $m - 1$ hyperplanes passing through the other nodes but not through the given nodes.

We start with some definitions, Let $\Theta = \{\theta_1, \dots, \theta_m\} \in \mathbb{R}^d$ be a set of points with some of the nodes possibly repeated. Here and in the following, Θ denotes a point set with some of the points possibly repeated, while Z is our old notation of a point set with no points repeated. Given an integrable function f on \mathbb{R}^d and a point set Θ , its *divided difference* $I_\Theta(f)$ of order $m - 1$ is defined to be

$$I_\Theta(f) = \int_0^1 \cdots \int_0^1 f(\theta_1 + s_1(\theta_2 - \theta_1) + \cdots + s_{m-1}(\theta_m - \theta_{m-1})) ds_{m-1} \cdots ds_1. \tag{37}$$

This is a direct generalization of the univariate divided difference (Eq. (16)) and leads to error estimates via remainder formulas (see [15, Section 2]).

For $z \in \mathbb{R}^d$ and f a continuously differentiable function on \mathbb{R}^d , the directional derivative, $D_z f$, of f in the direction z is denoted by

$$D_z f = z \cdot \nabla f.$$

To each $\lambda \in \mathbb{R}^d$, we associate the functional λ^* on \mathbb{R}^d defined by $\lambda^* z = \lambda \cdot z$ (the Euclidian scalar product).

A *plane wave*, or ridge function, h in \mathbb{R}^d is the composition of a functional and a univariate function $g : \mathbb{R} \rightarrow \mathbb{R}$

$$h(z) = (g \circ \lambda^*)(z) = g(\lambda^* z) \quad \text{for } z \in \mathbb{R}^d. \tag{38}$$

Let $C^s(\mathbb{R}^d)$ be the space of s times continuously differentiable functions on \mathbb{R}^d .

Now the main definition

Definition 20. Let $s \in \mathbb{N}_0$ be given and L associate with each finite set $\Theta \subset \mathbb{R}$ of points (possibly repeated) a continuous linear map L_Θ

$$L_\Theta : C^s(\mathbb{R}) \rightarrow C^s(\mathbb{R}).$$

A continuous linear map

$$\mathcal{L}_\Theta : C^s(\mathbb{R}^d) \rightarrow C^s(\mathbb{R}^d)$$

is the *lift* of L to $\Theta \subset \mathbb{R}^d$ if it satisfies

$$\mathcal{L}_\Theta(g \circ \lambda^*) = (L_{\lambda^* \circ g})\lambda^* \tag{39}$$

for any $\lambda \in \mathbb{R}^d$ and any $g \in C^s(\mathbb{R}^d)$. Here $\lambda^* \Theta = \{\lambda^* \theta_1, \dots, \lambda^* \theta_m\} \subset \mathbb{R}$ for $\Theta \subset \mathbb{R}^d$.

Since it is by no means clear that each map L has a lift, for example the univariate finite difference map has no lift, we say that L is *liftable* if it has a lift to each set Θ of point in \mathbb{R}^d . A lift, if it exists, is unique.

The maps we want to lift are Lagrange and Hermite maps. Given a node set $Z = \{z_1, \dots, z_m\} \subset \mathbb{R}$ and $g \in C(\mathbb{R})$, the Lagrange map $L_Z g$ delivers the interpolant to g from Π_{m-1}^1 . More generally, the Hermite map H_Θ based on the univariate Hermite interpolation given by (11) and (12) associates with each $g \in C^n(\mathbb{R})$, the Hermite interpolant from Π_n^d to the values $c_{q,\alpha} = D^\alpha g(z_q)$. Here, Z is the set of distinct points in Θ and k_q are their multiplicities. g was required to be in $C^n(\mathbb{R})$ with $n = \sum_{q=1}^m (k_q + 1) - 1$ since potentially all the points in Θ could coincide. Note also that the Hermite map becomes the Lagrange map when all the points of Θ are distinct.

The lift \mathcal{L} of say the Lagrange map would necessarily associate to each node set $Z \subset \mathbb{R}^d$ and function $f \in C(\mathbb{R})$ a multivariate polynomial from Π_{m-1}^d . In fact, let $f \in C(\mathbb{R}^d)$. Then f can be approximated arbitrarily well by linear combinations of plane waves. Since, by definition, \mathcal{L}_Θ is continuous, $\mathcal{L}_\Theta(f)$ can be approximated arbitrarily well by linear combinations of functions of the form $(L_{\lambda^* \circ g}) \circ \lambda^*$. But each $(L_{\lambda^* \circ g})$ is a univariate polynomial (in Π_{m-1}^1) and, consequently, so is $\mathcal{L}_\Theta(f)$ as their limit.

For the same reason, a lift \mathcal{H}_Θ of the Hermite map would also map $C^s(\mathbb{R}^d)$ to Π_n^d .

Before we formulate the general theorem on lifting Hermite maps, let us describe their precursors. Kergin (see [25]) first constructed a lift of the Hermite map but without using the concept of lifting.

Theorem 21. *Given a set of not necessarily distinct points $\Theta = \{\theta_1, \dots, \theta_{n+1}\}$ from \mathbb{R}^d , there exists a unique linear map $\mathcal{H}_\Theta : C^n(\mathbb{R}^d) \rightarrow \Pi_n^d$ such that for each $f \in C^n(\mathbb{R}^d)$, each $Q \in \Pi_k^d$, $0 \leq k \leq n$ and each $J \subset \{1, \dots, n+1\}$, there is a $z \in \text{span}\{\theta_q\}_{q \in J}$ such that*

$$Q(D)(\mathcal{L}_\Theta(f) - f)(z) = 0.$$

Choosing $J = \{q\}$ in this theorem shows that $\mathcal{H}_\Theta(f)(\theta_q) = f(\theta_q)$, so that \mathcal{H}_Θ indeed interpolates function values. Similarly, if θ_q is repeated k_q times, then all partial derivatives of f up to order k_q are interpolated at θ_q .

Micchelli, respectively, Micchelli and Milman [29,30] showed how to construct the Kergin interpolant by showing that it interpolates the functionals

$$f(\theta_1), I_{\{\theta_1, \theta_2\}}(\partial f / \partial x_i), \quad i = 1, \dots, d,$$

$$\dots, \quad I_{\{\theta_1, \dots, \theta_{n+1}\}}(D^\alpha f) \quad |\alpha| = n.$$

This is not such a nice representation of the functionals since, first of all, it is not clear from the formula that the interpolant is independent of the order in which the points θ_q are arranged and, secondly, it assumes an order of differentiability of f which is not really necessary. In fact, as was remarked in the original papers, it is independent of the choice of the nodes and, if the nodes are in general position, then Kergin’s interpolant has a continuous extension from $C^n(\mathbb{R}^d)$ to $C^{d-1}(\mathbb{R}^d)$.

To elucidate this, let us look Lagrange interpolation at three noncollinear nodes $\{\theta_1, \theta_2, \theta_3\}$ in \mathbb{R}^2 . The Kergin interpolant is from Π_2^2 whose dimension is 6. According to the representation given above, the functionals to be interpolated are $f(\theta_1)$, the average values of $\partial f / \partial x$ and $\partial f / \partial y$ along the line joining z_1 with z_2 , and the average values of $\partial^2 f / \partial x^2$, $\partial^2 f / \partial x \partial y$ and $\partial^2 f / \partial y^2$ over the triangle formed by the nodes. In [28], it was shown that one obtains the same interpolation if one interpolates the functionals $f(z_q)$, $q = 1, 2, 3$ and the average values of $\partial f / \partial n_i$ over the i th side of the triangle, $i = 1, 2, 3$. Here, n_i is the normal to the i th side. This representation is symmetric in the nodes and one sees that only $f \in C^1(\mathbb{R}^2)$ is required instead of $C^2(\mathbb{R}^2)$. Waldron [44] gives explicit formulas for the general case.

Interpolating average values of functions or their derivatives is not as exotic as it may seem. For example, a well-known finite element, the Wilson brick (see [7]), interpolates average values of second derivatives.

Another generalization of univariate Hermite interpolation to \mathbb{R}^d was given by Hakopian [21]. Let $\Theta \subset \mathbb{R}^d$ have $m \geq d + 1$ nodes in general position, meaning that any $d + 1$ of them form a nondegenerate tetrahedron. Then the problem of interpolating the functionals

$$I_{\tilde{\Theta}} \quad \text{for all } \tilde{\Theta} \subset \Theta \text{ with } |\tilde{\Theta}| = d$$

for $f \in C(\mathbb{R}^d)$ with polynomials from Π_{m-d}^d is regular. Here $|\Theta|$ is the cardinality of Θ . Note that there are exactly

$$\binom{m}{d}$$

interpolation conditions, which is also the dimension of Π_{m-d}^d .

Take three noncollinear nodes z_1, z_2, z_3 in \mathbb{R}^2 . Hakopian’s interpolant interpolates the average value of a function over the three sides of the triangle formed by the nodes.

Goodman [19] showed that these two types of interpolations are the end points of a whole scale of univariate Hermite interpolations, which are all liftable.

Let $f \in C(\mathbb{R})$ and let $D^{-r}f$ be any function with $D^r(D^{-r}) = f$. Then the generalized Hermite map $H_\Theta^{(r)}$ associated with r and the set $\Theta \subset \mathbb{R}$, with $|\Theta| = n + 1$, is the map

$$H_\Theta^{(r)} : C^{n-r}(\mathbb{R}) \rightarrow \Pi_{n-r}^1$$

given by

$$H_\Theta^{(r)} f = D^r H_\Theta D^{-r} f.$$

Theorem 22. For any r, n with $0 \leq r \leq n$, $H_{\Theta}^{(r)}$, with $|\Theta| = n + 1$, is liftable to $\mathcal{H}_{\Theta}^{(r)} : C^{n-r}(\mathbb{R}^d) \rightarrow \Pi_{n-r}^d$. The functionals interpolated are

$$I_{\Theta}(P_{\ell}(D)f) \tag{40}$$

for all $\tilde{\Theta} \subset \Theta$ with $|\tilde{\Theta}| \geq r + 1$ and where $\{P_{\ell}\}$ is a basis for the homogeneous d -variate polynomials of degree $|\tilde{\Theta}| - r - 1$.

If $r = 0$, we obtain the Kergin map. If $r = d - 1$, $n \geq d - 1$ and the points of Θ are in general position, we get the Hakopian map.

4.2. The least interpolant

Would it not be nice if given any functionals $F_q, q = 1, \dots, m$, we could find a polynomial space V such that the equations

$$F_q P = c_q, \quad q = 1, \dots, m$$

have a unique solution $P \in V$ for any c_q ? Note that the point of view has changed here. Given the functionals, we do not know which interpolation space to use, we derive it.

Well, if one is not too choosy, such a space almost always exists. All one needs is that the functionals be linearly independent in the space of all polynomials. Then a simple elimination argument shows that there are polynomials Q_r (dual polynomials) so that $F_q Q_r = \delta_{q,r}$. The linear span of these polynomials forms a possible space V .

The above construction is clearly not unique. One can require the interpolation space to have desirable properties. It turns out that the condition that the degree of the interpolant be as low as possible is a key concept, connecting the quest for good interpolation spaces with, among other things, Gröbner bases of polynomial ideals. This connection will be explained for Lagrange interpolation. Let $Z = \{z_1, \dots, z_m\}$ be a set of nodes in \mathbb{R}^d and V a space of polynomials from which Lagrange interpolation is regular. V is called degree reducing (the interpolant from V is degree reducing) if for any polynomial P , its interpolant Q satisfies $\deg Q \leq \deg P$.

A set of polynomials $\{P_{\alpha} | \alpha \in I \subset \mathbb{N}^d\}$ is called a Newton basis with respect to Z if Z can be indexed as $\{z_{\alpha} | \alpha \in I\}$ so that for any $\alpha, \beta \in I$ with $|\alpha| \leq |\beta|$, one has $P_{\alpha}(z_{\beta}) = \delta_{\alpha,\beta}$ and for any n , there is a decomposition

$$\Pi_n^d = \text{span}\{P_{\alpha} | |\alpha| \leq n\} \oplus \{Q \in \Pi_n^d | Q(z_q) = 0, q = 1, \dots, m\}.$$

Sauer [35] shows that

Theorem 23. A space of polynomials V has a Newton basis with respect to Z if and only if it is degree reducing for Z .

Even degree reducing spaces are not unique except when $V = \Pi_n^d$ for some n . These ideas can be generalized to Hermite interpolation and to orderings of Π^d which are compatible with addition, see [15,35, Section 3].

A closely related subject is that of Gröbner bases and H-bases. Let \prec be a total ordering of \mathbb{N}^d which has 0 as its minimal element and is compatible with addition (in \mathbb{N}^d). We will use it to order

the terms of a polynomial for which reason we call it a term order. Let I be an ideal of polynomials. A finite set \mathcal{P} is called a Gröbner basis for I if any polynomial $Q \in I$ can be written as

$$Q = \sum_{P \in \mathcal{P}} Q_P P,$$

where the (term order) degree of any summand does not exceed the degree of Q . If the term order degree is replaced by total degree, then we have an H-basis.

Now suppose I is the ideal associated with the node set Z , i.e., $I = \{P \mid P(z_q) = 0, q = 1, \dots, m\}$ and \mathcal{P} a Gröbner or an H-basis for I . Given a set of values to interpolate, let Q be any polynomial which interpolates them. We really want an interpolant of lowest possible degree (in our chosen ordering), so if the degree of Q is too high, we can eliminate the term of highest degree with some polynomial multiple of one of the basis polynomials. Continuing, we reduce Q as much as possible, arriving at a “minimal degree interpolant” with respect to the order used. This also works the other way around. One orders monomials according to some term order. Then one uses Gaussian elimination to find an interpolant. During the elimination, one encounters zero columns. The linear combinations producing these columns are just the coefficients of a Gröbner or an H-basis polynomial. We again refer to the survey paper [15] for the precise formulations of the above sketchy ideas. Other sources are Sauer [35,36], Buchberger [3], and Groebner [20].

The least interpolant of de Boor and Ron [8], which we will define now, is such a degree reducing interpolant. It uses an ordering of degrees “in blocks” of total degree.

Definition 24. Let g be a real-analytic function on \mathbb{R}^d (or at least analytic at $z = 0$)

$$g(z) = \sum_{|j|=0}^{\infty} a_j z^j.$$

Let j_0 be the smallest value of $|j|$ for which some $a_j \neq 0$. Then the *least term* of g is

$$g_{\downarrow} = \sum_{j=j_0} a_j z^j.$$

Note that g_{\downarrow} is a homogeneous polynomial of degree j_0 .

Theorem 25. Given a node set $Z \subset \mathbb{R}^d$, let

$$\text{Exp}_Z = \text{span}\{e^{z \cdot z_q} \mid q = 1, \dots, m\}$$

and

$$\mathcal{P}_Z = \text{span}\{g_{\downarrow} \mid g \in \text{Exp}_Z\}.$$

Then Lagrange interpolation from \mathcal{P}_Z to values at Z is regular.

The map $L : C(\mathbb{R}^d) \rightarrow \mathcal{P}_Z$ with Lf being the interpolant to the values of f on Z is called the least Lagrange interpolant. Note that $\dim \mathcal{P}_Z = \dim \text{Exp}_Z$.

Let us now look at some examples in \mathbb{R}^2 . First, let $Z = \{(0,0), (1,0), (0,1)\}$. We know that Lagrange interpolation from Π_1^2 at these nodes is regular. What does the least interpolant look like?

We have

$$\text{Exp}_Z = \text{span}\{e^0, e^x, e^y\} \\ = \left\{ (a + b + c) + bx + cy + b \sum_{j=2}^{\infty} \frac{x^j}{j!} + c \sum_{j=2}^{\infty} \frac{y^j}{j!} \mid a, b, c \in \mathbb{R} \right\}$$

so that

$$\mathcal{P}_Z = \text{span}\{1, x, y\} = \Pi_1^2.$$

If the nodes are collinear, say $Z = \{(0, 0), (1, 0), (2, 0)\}$, we get

$$\text{Exp}_Z = \text{span}\{e^0, e^x, e^y\} \\ = \left\{ (a + b + c) + (b + 2c)x + (b + 4c)x^2 + \sum_{j=3}^{\infty} (b + 2^j c) \frac{x^j}{j!} \mid a, b, c \in \mathbb{R} \right\}$$

so that

$$\mathcal{P}_Z = \text{span}\{1, x, x^2\},$$

which is the correct *univariate* space for Lagrange interpolation on three nodes on a line.

For the general case, we require that the functionals F_q be of the form $P(D)(z_q)$, where $P \in \Pi^d$ is a polynomial and $z_q \in \mathbb{R}^d$. Then the formal power series associated with a functional F is

$$g_F(z) = F(e^{y \cdot z}) := \sum_{|j|=0}^{\infty} \frac{F(y^j)}{j!} z^j.$$

The power series is called formal, since there is no convergence assumption. For the point evaluation functional $F(f) = f(z_q)$, we get $g_{F_q}(z) = e^{z \cdot z_q}$.

Now we can write down the interpolation space matching the functionals $\{F_q\}$

Theorem 26. Let $\mathcal{F} = \{F_1, \dots, F_m\}$ be functionals defined on Π^d . Let

$$\mathcal{G}_{\mathcal{F}} = \text{span}\{g_{F_1}, \dots, g_{F_m}\}$$

and

$$\mathcal{P}_{\mathcal{F}} = \text{span}\{g_{\downarrow} \mid g \in \mathcal{G}_{\mathcal{F}}\}.$$

Then for any values c_q , $q = 1, \dots, m$, there is exactly one $p \in \mathcal{P}_{\mathcal{F}}$ with

$$F_q(p) = c_q, \quad q = 1, \dots, m.$$

As an example, let us take our favorite singular Hermite interpolation. The functionals are evaluation of function values and the two first partial derivatives at z_1 and z_2 . To simplify computations, we take $Z = \{(0, 0), (1, 0)\}$.

To evaluate the power series, we use

$$\frac{\partial}{\partial x} e^{xx_q + yy_q} = x e^{z \cdot z_q}, \\ \frac{\partial}{\partial y} e^{xx_q + yy_q} = y e^{z \cdot z_q},$$

so that the power series are

$$e^0, xe^0, ye^0, e^x, xe^x, ye^x.$$

Doing the calculation as above, we get

$$\mathcal{P}_{\mathcal{F}} = \text{span}\{1, x, y, x^2, xy, x^3\}.$$

You can check for yourself that our Hermite interpolation from this space is regular. If we had taken nodes not lying on the coordinate axes, $\mathcal{P}_{\mathcal{F}}$ would no longer have a monomial basis.

Now that we have seen that it is relatively easy to construct the least interpolant, let us see what we are buying. By construction, we can now carry out Lagrange interpolation on any number of nodes without worrying whether the number matches a $\dim \Pi_n^d$. Other good properties of the least Lagrange interpolation on Z are that one can show that one has affine invariance in the sense that $\mathcal{P}_{aZ+z_0} = \mathcal{P}_Z$, for any real a and $z_0 \in \mathbb{R}$. Also one has transformation rules as for a change of variables: if A is a nonsingular $d \times d$ matrix, then $\mathcal{P}_{AZ} = \mathcal{P}_Z \cdot A^T$.

One of its most important properties is that the least interpolant is degree reducing. From this, it follows that if Lagrange interpolation on Z is regular for some complete space Π_n^d , then $\mathcal{P}_Z = \Pi_n^d$. Formulating this differently, if $Z \subset \mathbb{R}^d$, $m = \dim \Pi_n^d$ for some j and the functionals are the point evaluation functionals, then $\mathcal{P}_Z = \Pi_n^d$ a.e., since Lagrange interpolation is regular a.e.

This raises the question of the behavior of the spaces \mathcal{P}_Z when Z changes or what happens to \mathcal{P}_Z when two nodes coalesce. If two of the nodes coalesce along a straight line, it can be shown that the least Lagrange interpolant converges to the Hermite interpolant which replaces one of the functional evaluations at the coalesced node with the directional derivative in the direction of the line.

But the first question does raise some computational issues. If $m = \dim \Pi_n^d$ for some j , then the set of Z for which $\mathcal{P}_Z = \Pi_n^d$ is open in \mathbb{R}^{dm} . If Z moves to a location in which Lagrange interpolation is singular, \mathcal{P}_Z must change discontinuously. Thus, around this location, computation of a basis for \mathcal{P}_Z is unstable. This is not to say that classical polynomial interpolation is better in this regard. It is even worse: the interpolant just does not exist for those Z . That this problem can be solved computationally is show by de Boor and Ron in [9]. They have have also developed a MATLAB program implementing these ideas.

5. Explicit interpolation schemes

5.1. Introduction

In this section, we will discuss two types of interpolation schemes. The first is to find concrete locations of points for which classical Lagrange interpolation is regular. The second is to construct Hermite interpolations, including the node sets, guaranteed to be regular. These are usually not of the classical type, but they have certain advantages. For example, some of them can be computed in a Newton like way.

5.2. Explicit Lagrange interpolation schemes

Chung and Yao, [6], give a quasi-constructive description of locations of nodes in \mathbb{R}^d for which Lagrange interpolation is regular. They satisfy the

Definition 27. A node set $Z = \{z_1, \dots, z_m\} \subset \mathbb{R}^d$ with $m = \dim \Pi_n^d$ for some n is said to satisfy the *General Condition* if to each node z_q , there exist n hyperplanes $H_{q,1}, \dots, H_{q,n}$ such that

- (a) z_q does not lie on any of these hyperplanes,
- (b) all other nodes lie on at least one of them.

A node set satisfying the general condition is said to be a *natural lattice*. It can easily be shown that Lagrange interpolation from Π_n^d on a natural lattice is regular since the n functions

$$\lambda_q(z) := \frac{\prod_{i=1}^n H_{q,i}(z)}{\prod_{i=1}^n H_{q,i}(z_q)}$$

are Lagrange fundamental functions. Here $H_{q,i}(z) = 0$ are the hyperplanes required by the General Condition. This is very much in the spirit of the univariate construction in Eq. (14). This idea has been extended to Hermite interpolation by Busch, see [4].

Finding regular Lagrange interpolations via natural lattices is not really constructive. It is actually just a sufficient condition for regularity. However, it has been the motivation for several explicit constructions. Let us first look at triangular arrays

$$Z_n^d := \{j \mid j \in \mathbb{N}_0^d, |j| \leq n\}.$$

With a little bit of work, one can convince oneself that each Z_n^d satisfies the general condition (do not forget the hyperplanes perpendicular to the direction $(1, \dots, 1)$!)

A nicer example in \mathbb{R}^2 , worked out in great detail by Sauer and Xu, [39], starts with $2r + 1$ points equi-distributed on the circumference of the unit disk. We number the points z_1, \dots, z_{2r+1} and connect z_q with z_{q+r} by a straight line. Here, $q + r$ is taken modulo $2r + 1$. Let $Z^{(r)}$ be the set of intersections of these lines within and on the circumference of the circle. Then it can be shown that

Theorem 28. *The node set $Z^{(r)}$ described above contains exactly $r(2r + 1) = \dim \Pi_{2r-1}^2$ points. It is a natural lattice and, consequently, Lagrange interpolation on $Z^{(r)}$ from Π_{2r-1}^2 is regular.*

Due to the concrete location of the nodes, they lie on r concentric circles, Sauer and Xu are able to give compact formulas for the fundamental functions and a point-wise bound for the error of the interpolant. Bos [2] has some similar constructions which we discuss in Section 4.

Now, let us look at a really constructive approach to Lagrange interpolation given by Gasca and Maeztu [11]. Let there be given $n + 1$ distinct lines $\ell_i(z) = 0$, $i = 0, \dots, n$. To each line ℓ_i , we associate lines $\ell_{i,j}$, $j = 0, \dots, r(i)$ each of which intersect ℓ_i at exactly one point $z_{i,j}$. In addition, it is assumed that the node $z_{i,j}$ does not lie on any of the lines $\ell_0, \dots, \ell_{i-1}$, $1 \leq i \leq n$. Sets of lines satisfying these conditions are called admissible.

We set

$$Z = \{z_{i,j} \mid 0 \leq j \leq r(i), 0 \leq i \leq n\}. \tag{41}$$

Now we must define the space from which we will interpolate. Let

$$P_{0,0}(z) = 1, \tag{42}$$

$$P_{0,j}(z) = \ell_{0,0} \cdots \ell_{0,j-1}(z), \quad 1 \leq j \leq r(0), \tag{43}$$

$$P_{i,0}(z) = \ell_0 \cdots \ell_{i-1}(z), \quad 1 \leq i \leq n, \tag{44}$$

$$P_{i,j}(z) = \ell_0 \cdots \ell_{i-1}(z) \ell_{i,0} \cdots \ell_{i,j-1}(z), \quad 1 \leq j \leq r(i), 1 \leq i \leq n. \tag{45}$$

Then we set

$$V = \text{span}\{P_{i,j} \mid 0 \leq j \leq r(i), 0 \leq i \leq n\}. \tag{46}$$

Theorem 29. *Lagrange interpolation on Z given by (41) from V given by (46) is regular.*

How to prove this theorem becomes clear once we recognize that (42) and the following equations can be given recursively by

$$P_{i,0}(z) = P_{i-1,0}(z) \ell_{i-1}(z), \quad 1 \leq i \leq n,$$

$$P_{i,j}(z) = P_{i,j-1}(z) \ell_{i,j-1}(z), \quad 1 \leq j \leq r(i), 1 \leq i \leq n.$$

If we order the nodes of Z lexicographically, that is $(i, j) < (i', j')$ if $i < i'$ or if $i = i'$, then $j < j'$, it is easy to see from the above recursive construction that

$$P_{i',j'}(z_{i,j}) = 0 \quad \text{if } (i, j) < (i', j').$$

If Z is admissible, $P_{i,j}(z_{i,j}) \neq 0$. Thus the interpolant can be constructed exactly as in the univariate Newton construction of Section 2.1.

Many people have considered the special case that the lines ℓ_i are taken parallel to the x -axis. Then the lines $\ell_{i,j}$ can be taken parallel to the y -axis.

What does the interpolation space look like? First, we must note that many different admissible choices of lines can lead to the same node set. Thus we can have many different spaces for the same functionals. In one special, but very important case, V is independent of the lines. This is the case when we would like to have $V = \Pi_n^2$ for some n . To achieve this, we choose $r(i) = n - i$, $0 \leq i \leq n$ and the lines so that the admissibility condition is satisfied. Then $\dim V = \dim \Pi_n^2$. But, by Theorem 29, all the polynomials in (42) are linearly independent and, from (42), it can be seen that each of them is of degree not exceeding n . Thus $V = \Pi_n^2$ as desired, independently of the choice of lines.

Comparing their results with those of Chung and Yao, Gasca and Maeztu have made the conjecture.

Conjecture 30. *Let Z be a natural lattice in \mathbb{R}^2 for some n . Then one of the lines involved in the definition of the general condition contains exactly $n + 1$ nodes of Z .*

Note that no line can contain more than $n + 1$ nodes, since then Lagrange interpolation will not be regular.

If the conjecture were true, then we could remove those $n + 1$ nodes obtaining a smaller node set $Z^{(1)}$, which satisfies the general condition with respect to Π_{n-1}^2 . Continuing in this way, we could

conclude that any natural lattice is a special case of the above construction of Gasca and Maeztu for obtaining interpolation spaces with $V = \Pi_n^2$.

Gasca and Maeztu’s construction has a straightforward generalization to \mathbb{R}^d , leading to a Newton formula for Lagrange interpolation in \mathbb{R}^d . Their method also includes Hermite interpolation. This will be presented in the following subsection.

The final type of construction we mention here can be subsumed under the concept of “Boolean sum”. A detailed exposition of this class of constructions, which can also be used for trigonometric polynomials, can be found in a book by Delvos and Shempp [10].

The simplest example of such interpolations is called Biermann interpolation. It is based on univariate interpolation and the boolean sum of two commuting projectors. Let L and M be two commuting projectors. Then their *boolean sum* $L \oplus M$ is given by

$$L \oplus M = L + M - LM.$$

The projectors we use are those of univariate Lagrange interpolation

$$(L_n f)(x) = \sum_{q=1}^{n+1} f(x_q) \lambda_{q,n}(x) \quad \text{for } f \in C(\mathbb{R}), \tag{47}$$

where $\lambda_{q,n}$ are the Lagrange fundamental functions for interpolation from Π_n^1 on $X = \{x_1, \dots, x_{n+1}\}$. These projectors are extended to $C(\mathbb{R}^2)$ by just applying them to one of the variables

$$(L_n f)(x, y) = \sum_{q=1}^{n+1} f(x_q, y) \lambda_{q,n}(x) \quad \text{for } f \in C(\mathbb{R}^2). \tag{48}$$

By M_s , we denote the same projector, but now applied to the y variable and based on the node set $Y = \{y_1, \dots, y_{s+1}\}$. Then L_n and M_s commute and

$$(L_n M_s f)(x, y) = \sum_{p=1}^{n+1} \sum_{q=1}^{s+1} f(x_p, y_q) \lambda_{p,n}(x) \lambda_{q,s}(y) \quad \text{for } f \in C(\mathbb{R}^2).$$

Choose now increasing integer sequences $1 \leq j_1 < \dots < j_r$; $1 \leq l_1 < \dots < l_r$ and nodes $X = \{x_1, \dots, x_{j_r+1}\}$, $Y = \{y_1, \dots, y_{l_r+1}\}$. Then the Biermann projector is defined by

$$B_r = L_{j_1} M_{l_r} \oplus L_{j_2} M_{l_{r-1}} \oplus \dots \oplus L_{j_r} M_{l_1}. \tag{49}$$

The interpolation space is defined similarly

$$V = \Pi_{(j_1, l_r)} + \Pi_{(j_2, l_{r-1})} + \dots + \Pi_{(j_r, l_1)}. \tag{50}$$

Here the sum of two subspaces U and V is defined by $U + V = \{u + v \mid u \in U, v \in V\}$.

Theorem 31. *Lagrange interpolation from V given in (50) on the node set*

$$Z = \{(x_i, y_j) \mid 1 \leq i \leq j_m + 1, 1 \leq j \leq l_{r+1-m} + 1, 1 \leq m \leq r\}$$

is regular. The interpolation is given explicitly by

$$(B_r f)(x, y) = f(x_i, y_j)$$

where B_r is the Biermann projector (49).

The interpolation space has a monomial basis, so if we write $V = \Pi_A$, then A resembles (optically) the node set. Both have the same cardinality

$$\sum_{m=1}^r (k_m + 1)(l_{r+1-m} - l_{r-m}).$$

The special case that $k_m = l_m = m - 1$ for $m = 1, \dots, r + 1$ turns out to be the Lagrange interpolation from Π_r^2 on the triangular array given in Section 2.2. The Biermann projector is defined similarly in higher dimensional euclidean spaces.

One of the nice features of these kinds of interpolations is that the error of interpolation can be expressed as a product of the univariate errors.

5.3. Explicit Hermite interpolation schemes

Gasca and Maeztus technique for Lagrange interpolation given in the previous subsection can be used to obtain Hermite interpolation simply by dropping the assumption the lines need be distinct, and that the intersection $z_{i,j}$ of ℓ_i and $\ell_{i,j}$ not lie on any of the lines “preceding” it in the sense mentioned in the previous subsection. The definition of the interpolating space remains the same as before (42), (46), but with the lines repeated according to their multiplicities. But the functionals to be interpolated change. This is to be Hermite interpolation after all. To describe them, we use the notation previously introduced. Let t_i be lines orthogonal to ℓ_i and $t_{i,j}$ be lines orthogonal to $\ell_{i,j}$. We define the numbers

$$a_i = \begin{cases} 0 & \text{if } j = 0, \\ \text{the number of lines among} \\ \{\ell_0, \dots, \ell_{i-1}\} \text{ coincident with } \ell_i & \text{if } 1 \leq i \leq n, \end{cases} \tag{51}$$

$$b_i = \begin{cases} 0 & \text{if } i = 1, \\ \text{the number of lines among} \\ \{\ell_0, \dots, \ell_{i-1}\} \text{ that contain } z_{i,j} & \text{if } 1 \leq i \leq n, \end{cases} \tag{52}$$

$$c_{i,j} = \begin{cases} 0 & \text{if } j = 0, \\ \text{the number of lines among} \\ \{\ell_{i,0}, \dots, \ell_{i,j-1}\} \text{ that contain } z_{i,j} & \text{if } 1 \leq j \leq r(i). \end{cases} \tag{53}$$

The functionals to be interpolated are

$$D_{i,j}f = D_i^{a_i} D_{i,j}^{b_i+c_{i,j}} f(z_{i,j}), \quad 1 \leq i \leq n, \quad 1 \leq j \leq r(i), \tag{54}$$

where, as before, $D_t f$ is the directional derivative of f in the direction t .

Theorem 32. *The interpolation of the functionals (54) from the space spanned by the polynomials (42) is regular.*

For another approach which yields regular interpolation schemes similar in flavor to those just discussed, see Gevorkian et al. [17]. There $V = \Pi_n^d$ and they obtain their interpolation conditions by projections onto the intersection of families of hyperplanes.

If we start with a Hermite interpolation, then it seems clear that one obtains another by subjecting all components, the node set and the interpolation space to an affine transformation. This was carried out systematically by Gasca and Mühlbach in [12–14]. There starting with a node set lying on a Cartesian grid, they apply projectivities to obtain new schemes. For these new schemes, one can find Newton-type interpolation formulas and formulas for the error of interpolation resembling the univariate ones. These projectivities allow mapping “finite” points to “infinity” and thus one can obtain nodes lying on pencils of rays. This extends an approach used by Lee and Philips [26].

5.4. Node sets on algebraic varieties

The interpolation schemes presented in the previous subsections were very much concerned with lines and hyperplanes. In this subsection, we look at Lagrange interpolation on node sets restricted to algebraic varieties. The presentation is taken from Bos [2]. By *algebraic variety* or algebraic manifold, we mean sets of the form

$$W = \{z \in \mathbb{R}^d \mid P(z) = 0, P \in \mathcal{P}\}, \tag{55}$$

where \mathcal{P} is a collection of polynomials from Π^d . Given a point set $E \subset \mathbb{R}^d$, the *ideal* I_E associated with E is

$$I_E = \{P \in \Pi^d \mid P(z) = 0, z \in E\}. \tag{56}$$

If E is a variety, then we say that I_E is the *ideal of the variety*. An ideal is called *principal* if there is a $Q \in \Pi^d$ such that

$$I = \{PQ \mid P \in \Pi^d\}. \tag{57}$$

Finally, given a point set $E \subset \mathbb{R}^d$,

$$N_n^d(E) = \dim(\Pi_n^d|_E).$$

Much of the following is based on the

Lemma 33. *Let W be an algebraic variety whose ideal I_W is principal being represented by the polynomial Q . Then*

$$N_n^d(W) = \binom{n+d}{d} - \binom{n - \deg Q + d}{d}.$$

In the following, we fix n, d and want to interpolate from Π_n^d .

Let W_1, \dots, W_N be algebraic varieties whose ideals are principal and are represented by the polynomials Q_1, \dots, Q_N having degrees n_1, \dots, n_N . Assume that these polynomials are pairwise relatively prime and, in addition,

$$n_1 + \dots + n_{N-1} < n, \tag{58}$$

$$n_1 + \dots + n_N \geq n. \tag{59}$$

Set $s_i = n - n_1 - \dots - n_{i-1}$ and let Z_i be an arbitrary set of $N_{s_i}^d$ points on W_i , $i = 1, \dots, N$ such that all of these points are distinct. If $n_1 + \dots + n_N > n$, set

$$Z = \bigcup_{i=1}^N Z_i \tag{60}$$

and if $n_1 + \dots + n_N = n$, put

$$Z = \bigcup_{i=1}^N Z_i \cup \{a\}, \tag{61}$$

where a does not lie on any of the W_i . With this choice, there are always a total of $\dim \Pi_n^d$ nodes in Z .

The reason for choosing the nodes this way is that the regularity of Lagrange interpolation on Z can be decomposed to the Lagrange regularity on each of the varieties.

Theorem 34. *Let $Z, Z_i, i = 1, \dots, N$, be chosen as above. If Lagrange interpolation from $\Pi_{s_i}^d|_{W_i}$ on Z_i is regular for $i = 1, \dots, N$, then Lagrange interpolation from Π_n^d on Z is regular.*

This theorem is proved by repeated application of Lemma 33.

For a simple example of this technique, we consider varieties which are concentric circles in \mathbb{R}^2 . Take distinct radii $R_i, i = 1, \dots, N$, and

$$W_i = \{(x, y) \mid x^2 + y^2 = R_i^2\}.$$

Then each I_{W_i} is a principal ideal with $P_i = x^2 + y^2 - R_i^2$, so $n_i = 2$. We fix n and want to interpolate from Π_n^2 . By (58) and (59), we must choose $N = [(n + 1)/2]$, where $[a]$ is the integer part of a . Then $n_1 + \dots + n_N > n$ if n is odd and $n_1 + \dots + n_N = n$ if n is even. It follows that $s_i = n - 2(i - 1)$ and that, by Lemma 33, that

$$N_{s_i}^d(W_i) = \binom{s_i + 2}{2} - \binom{s_i - 2 + 2}{2} = 2s_i + 1.$$

But Lagrange interpolation by algebraic polynomials of degree s_i on $2s_i + 1$ nodes on a circle centered at the origin is the same as interpolation by trigonometric polynomials of the same degree, which is regular. So taking an additional point $(0, 0)$ in n is even, Theorem 34 allows us to conclude that Lagrange interpolation from Π_n^d on a node set consisting of $2n - 4i + 5, i = 1, \dots, N$ nodes lying respectively on $N = [(n + 1)/2]$ concentric circles, is regular.

The Lagrange interpolation by Sauer and Xu mentioned in Section 5.2 is also has its nodes lying on concentric circles. In that construction, there are $r(r + 1)$ nodes when interpolating from Π_{2r-1}^2 . These nodes are distributed over r circles, with $r + 1$ nodes on each of them. In the example of Bos, the number of nodes on the circles differs from circle to circle, but their location on the circles can be chosen at will. Another difference is that the circles given by Sauer and Xu have the predetermined radii

$$R_j = \frac{\cos j\pi/(2j + 1)}{\cos r\pi/(2j + 1)}, \quad j = 1, \dots, r.$$

Despite the resemblance, it does not seem that there is any connection between these schemes.

As we have seen in this and the previous section, the study of polynomial ideals is quite useful for multivariate interpolation. More about them can be found in Möller [32,33], Xu [45] and the references given in Section 4.

6. Related topics

6.1. Introduction

In this section, we will look at the theory of singularities, i.e., at the investigation of the set of polynomials having zeros of given multiplicities. The last subject will be the results of Vassiliev on the minimal dimension an interpolation space must have in order to be able to solve a Lagrange interpolation for any choice of nodes.

6.2. Singularities

In concordance with the notation generally used, we will speak of singularities of a given order of a function. A function f defined on \mathbb{R}^d has a *singularity of order s* at z if

$$D^\alpha f(z) = 0 \quad \text{for } |\alpha| < s.$$

On the other hand, we consider polynomials in euclidian and not in projective spaces, so that some of our notation does differ for example from the survey paper of Miranda [31], from which some of this material was taken. Let $Z = \{z_1, \dots, z_m\}$ be a set of nodes in \mathbb{R}^d and $\{s_1, \dots, s_m\} \subset \mathbb{N}^d$. Then $\mathcal{L}_n^{(d)}(-\sum_{q=1}^m s_q z_q)$ stands for the subspace of Π_n^d of polynomials having a singularity of order s_q at z_q for $q = 1, \dots, m$. $\mathcal{L}_n^{(d)}(-\sum_{q=1}^m s_q z_q)$ could consist of just the zero polynomial or be very large, since there is no connection between the number of singularities and the degree of the polynomials. The *virtual dimension* $v_n^{(d)}$ of $\mathcal{L}_n^{(d)}(-\sum_{q=1}^m s_q z_q)$ is

$$v_n^{(d)} \left(-\sum_{q=1}^m s_q z_q \right) = \binom{d+n}{d} - \sum_{q=1}^m \binom{s_q-1}{d}.$$

Intuitively, if we take Π_n^d and subject it to the

$$\sum_{q=1}^m \binom{s_q-1}{d}$$

conditions that the polynomials have the given singularities on Z , then we expect to reduce its dimension by exactly this number, unless this number is larger than the dimension of Π_n^d , in which case, we expect to get dimension 0. Thus, we define the *expected dimension* $e_n^{(d)}$ by

$$e_n^{(d)} \left(-\sum_{q=1}^m s_q z_q \right) = \max \left\{ 0, v_n^{(d)} \left(-\sum_{q=1}^m s_q z_q \right) \right\}.$$

What does this mean for an interpolation scheme? There

$$\binom{d+n}{d} = \sum_{q=1}^m \binom{s_q-1}{d}, \tag{62}$$

so that the expected dimension is always 0. If the true dimension is not 0, then there is a polynomial in Π_n^d which satisfies the homogeneous interpolation conditions. Thus the interpolation is singular.

As we have seen from Theorem 2, for each Hermite interpolation (except the Taylor interpolation) there are always node sets Z for which the dimension of $\mathcal{L}_n^{(d)}(-\sum_{q=1}^m s_q z_q)$ is nonzero, i.e., for which the interpolation is singular. This is nothing special. On the other hand, it is a rather special situation if the dimension of $\mathcal{L}_n^{(d)}(-\sum_{q=1}^m s_q z_q)$ is *always* larger than the expected dimension. Thus we say that the system of homogeneous equations described by $(n; s_1, \dots, s_m)$, whose solution yields $\mathcal{L}_n^{(d)}(-\sum_{q=1}^m s_q z_q)$ if solved for the node set Z , is *special* if

$$\inf_Z \dim \mathcal{L}_n^{(d)} \left(-\sum_{q=1}^m s_q z_q \right) > e_n^{(d)} \left(-\sum_{q=1}^m s_q z_q \right). \tag{63}$$

An example is the system $(2; 2, 2)$, which is our favorite singular Hermite interpolation. It is special. We have

$$\inf_Z \dim \mathcal{L}_2^{(2)} \left(-\sum_{q=1}^2 2z_q \right) = 1$$

while

$$e_2^{(2)} \left(-\sum_{q=1}^2 2z_q \right) = 0.$$

Nodes for which the minimum in (63) is attained are said to be in *general position*. This is not quite the usual definition, but is equivalent. Be aware of the fact that we have already used “general position” with another meaning.

So, the concept of special systems is wider than that of singular Hermite interpolations of type total degree. A special system which happens to be an interpolation, i.e., for which (62) holds, is a singular interpolation scheme.

It has been a problem of long standing in algebraic geometry to determine, or to characterize all special systems. They have come up with the following conjecture in \mathbb{R}^2 .

Conjecture 35. *Let $(n; s_1, \dots, s_m)$ be a special system in \mathbb{R}^2 and P a solution of it for some node set in general position. Then there is a (nonzero) polynomial Q such that Q^2 divides P . The polynomial Q is a solution of a system $(r; t_1, \dots, t_m)$ with the same nodes and with*

$$r^2 - \sum_{q=1}^m s_q = -1. \tag{64}$$

Hirschowitz [22,23] has verified this conjecture for some special cases

Theorem 36. *Let $n, d \geq 2$. The linear system $(n; 2, \dots, 2)$ with m nodes in \mathbb{R}^d is special exactly in the following cases:*

- (a) for $n = 2$: if and only if $2 \leq m \leq d$,
- (b) for $n \geq 3$: if and only if (d, n, m) is one of $(2, 4, 5)$, $(3, 4, 9)$, $(4, 3, 7)$ or $(4, 4, 14)$.

We have already seen some of these. Theorem 16, formulated in the terminology of this section, states that interpolations $(n; s_1, \dots, s_m)$ in \mathbb{R}^d are special if $2 \leq m \leq d + 1$. One must exercise care when comparing the two results, since the above theorem also includes non-interpolation schemes. For example, the systems described in a) are interpolating if and only if $m = 1 + d/2$, i.e., only for spaces of even dimension. In those cases, they are, indeed, covered by Theorem 16.

Of the special schemes in (b), $(2, 4, 5)$, $(4, 3, 7)$ and $(4, 4, 14)$ are interpolations. The scheme $(3, 4, 9)$ has 36 interpolation conditions, while the dimension of the interpolation space is 35. The singularity of $(2, 4, 5)$ and $(4, 4, 14)$ follow from Theorem 18.

There are many other results in the literature. For example, Hirschowitz [22], treats the case $(n; 3, \dots, 3)$ exhaustively.

Let us now return to the condition $n^2 - \sum_q s_q^2 = -1$ of Conjecture 35. It derives from the calculus on schemes we used in Section 3.3: addition is

$$(n_1; s_{1,1}, \dots, s_{1,m}) + (n_2; s_{2,1}, \dots, s_{2,m}) = (n_1 + n_2; s_{1,1} + s_{2,1}, \dots, s_{1,m} + s_{2,m})$$

and an “inner product” is

$$\langle (n_1; s_{1,1}, \dots, s_{1,m}), (n_2; s_{2,1}, \dots, s_{2,m}) \rangle = n_1 n_2 - \sum_{q=1}^m s_{1,q} s_{2,q}.$$

Thus if we set $\mathcal{N} = (n; s_1, \dots, s_m)$, then

$$n^2 - \sum_{q=1}^m s_q^2 = \langle \mathcal{N}, \mathcal{N} \rangle.$$

Many facts about interpolation schemes can be expressed in terms of this calculus. For example, if \mathcal{N}_1 and \mathcal{N}_2 are special then so is $\mathcal{N}_1 + \mathcal{N}_2$. In fact, if P_i are polynomials satisfying \mathcal{N}_i , $i = 1, 2$, then, as we have seen before, $P_1 \cdot P_2$ satisfies $\mathcal{N}_1 + \mathcal{N}_2$. Or, Bezout’s theorem (in \mathbb{R}^2) can be expressed in the following way: If P_i are polynomials satisfying \mathcal{N}_i , $i = 1, 2$ which are relatively prime, then

$$\langle \mathcal{N}_1, \mathcal{N}_2 \rangle \geq 0.$$

Here the schemes are not assumed to be special.

We can also reformulate Hirschowitz’ conjecture

Conjecture 37. *Let \mathcal{N} be a special interpolation scheme in \mathbb{R}^2 . Then there is another scheme \mathcal{R} satisfying condition (64) such that*

$$\langle \mathcal{N}, \mathcal{R} \rangle = -2.$$

More details about this calculus can be found in Miranda [31].

It is interesting to note, that Gevorkian Hakopian and Sahakian have a series of papers of singular Hermite interpolations, some of which we have already referred to, in which they use exactly this calculus, but with a slightly different notation. They have also formulated a conjecture about singular interpolations which is based on schemes which have fewer interpolation conditions than the dimension of the space being interpolated from. They say that $(n; s_1, \dots, s_1)$ belongs to the

less condition class (LC), if (in \mathbb{R}^2)

$$\binom{n+2}{2} > \sum_{q=1}^m \binom{s_q+2}{2}.$$

As we have seen, the importance of these “less” schemes is that there always exists a polynomial satisfying the homogeneous conditions, i.e., $\mathcal{L}_n^{(2)}(-\sum_{q=1}^m s_q z_q)$ has dimension at least one for each node set.

Their conjecture, reformulated in terms of special schemes, is

Conjecture 38. *Let \mathcal{N} be an interpolation scheme in \mathbb{R}^2 . Then \mathcal{N} is special if and only if there are schemes $\mathcal{M}_i, i = 1, \dots, r$ belonging to LC, such that*

$$\mathcal{N} = \sum_{i=1}^r \mathcal{M}_i.$$

This conjecture is not true in \mathbb{R}^3 : $\mathcal{N} = (4; 3, 3, 1, \dots, 1)$ with 15 1’s is a singular interpolation scheme in \mathbb{R}^3 which is not decomposable into “less” schemes.

No one seems to have integrated the results from these two sources.

6.3. Lagrange interpolation spaces of minimal dimension

In this subsection, we stay with Lagrange interpolation but allow interpolating spaces consisting of arbitrary functions. What we want to do is to fix the number of nodes and then find one interpolation space, such that Lagrange interpolation on that number of nodes is always solvable, no matter where the nodes are located. If the number of nodes is equal to the dimension of a complete space of polynomials (in \mathbb{R}^d for $d \geq 2$), then it is clear that we cannot choose that space itself. But perhaps there is another possibly non-polynomial space of the same dimension that does the trick. If not, then we allow the dimension of the space from which we will interpolate to increase until we have found one that works. The theorem of Severi (Theorem 19) tells us that if we want to do Lagrange interpolation on m nodes in \mathbb{R}^d , then we can do it with Π_{m-1}^d . Its dimension is

$$\binom{m-1+d}{d}.$$

If we allow noncomplete spaces of polynomials, then one can get away with smaller dimension. In [28], it is shown that it can be done with a space of dimension roughly $m \ln m$ in \mathbb{R}^2 . Vassiliev [42] has considered these questions in a more general context.

Let M be a topological space, V a finite dimensional subspace of $C(M)$ (not necessarily polynomial). V is called m -interpolating (over M) if the Lagrange interpolation problem: find $P \in V$ such that

$$f(z_q) = c_q, \quad q = 1, \dots, m \tag{65}$$

is solvable for any choice of nodes z_q from M and values c_q . Before, in the context of Severi’s theorem, we called the problem “solvable” in this case. Here $\dim V = m$ is not assumed and, in

general, not possible. Now we want to find the space of lowest possible dimension, and define

$$I(V, m) = \min_Z \dim V,$$

where the minimum is taken over all spaces which are m -interpolating and over all node sets Z of size m .

For example, $I(\mathbb{R}, m) = m - 1$ and a space of minimal dimension is Π_{m-1}^1 . A first interesting result by Vassiliev is

Theorem 39.

$$2m - b(m) \leq I(\mathbb{R}^2, m) \leq 2m - 1,$$

where $b(m)$ is the number of ones in the binary representation of m .

It immediately follows that, for example, that $I(\mathbb{R}^2, 2^n) = 2 \cdot 2^n - 1$, since $b(2^n) = 1$. For $m = 3$, $b(m) = 2$ and the lower bound is the true value. A space of minimal dimension is $V = \text{span}\{1, x, y, x^2 + y^2\}$. V is 3-interpolating. In fact, $V = \text{span}\{1, \Re z^t, \Im z^t \mid 1 \leq t \leq m - 1\}$, where $z = x + iy$, provides the upper bound in the theorem. The lower bound is the difficult one to prove.

If $M = S^1$ is the unit circle in \mathbb{R}^2 , then $I(M, m) = m$ if m is odd and $I(M, m) = m + 1$ if m is even, for we can take the space of trigonometric polynomials of degree $[m/2]$ in both cases.

Theorem 40. For any d -dimensional manifold M , we have

$$I(M, m) \leq m(d + 1).$$

In the case of the unit circle, the theorem predicts $2m$ instead of the correct answer $2[m/2] + 1$.

I suppose this theory has more conjectures than proven theorems, so, appropriately, we close with another conjecture of Vassiliev

Conjecture 41. If d is a power of 2, then

$$I(\mathbb{R}^d, m) \geq m + (d - 1)(m - b(m)).$$

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Interpolation by Cauchy–Vandermonde systems and applications

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Abstract

Cauchy–Vandermonde systems consist of rational functions with prescribed poles. They are complex ECT-systems allowing Hermite interpolation for any dimension of the basic space. A survey of interpolation procedures using CV-systems is given, some equipped with short new proofs, which generalize the well-known formulas of Lagrange, Neville–Aitken and Newton for interpolation by algebraic polynomials. The arithmetical complexity is $\mathcal{O}(N^2)$ for N Hermite data. Also, inversion formulas for the Cauchy–Vandermonde matrix are surveyed. Moreover, a new algorithm solving the system of N linear Cauchy–Vandermonde equations for multiple nodes and multiple poles recursively is given which does not require additional partial fraction decompositions. As an application construction of rational B-splines with prescribed poles is discussed. © 2000 Elsevier Science B.V. All rights reserved.

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1. Cauchy–Vandermonde systems; definitions and notations

Let

$$\mathcal{B} = (b_1, b_2, \dots) \tag{1}$$

be a given sequence of not necessarily distinct points of the extended complex plane $\bar{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. With \mathcal{B} we associate a system

$$\mathcal{U} = (u_1, u_2, \dots) \tag{2}$$

of basic rational functions defined by

$$u_j(z) = \begin{cases} z^{v_j(b_j)} & \text{if } b_j = \infty, \\ (z - b_j)^{-(v_j(b_j)+1)} & \text{if } b_j \in \mathbb{C}. \end{cases} \tag{3}$$

Here

$$v_j(b) \text{ is the multiplicity of } b \text{ in the sequence } (b_1, \dots, b_{j-1}). \tag{4}$$

The system \mathcal{U} has been called [18,17,15,13,12,5] the *Cauchy–Vandermonde system* (CV-system for brevity) associated with the pole sequence \mathcal{B} . By \mathbb{N} we denote the set of positive integers. For any fixed $N \in \mathbb{N}$ to the initial section of \mathcal{B}

$$\mathcal{B}_N = (b_1, \dots, b_N) \tag{5}$$

there corresponds the basis

$$U_N = (u_1, \dots, u_N) \tag{6}$$

of the N -dimensional *Cauchy–Vandermonde space* $\mathcal{U}_N := \text{span } U_N$. Indeed, for every $N \in \mathbb{N}$ U_N is an *extended complete Čebyšev system* on $\mathbb{C} \setminus \{b_1, \dots, b_N\}$. This follows from

Proposition 1. *For any system*

$$\mathcal{A} = (a_1, a_2, \dots) \tag{7}$$

of not necessarily distinct complex numbers a_i such that \mathcal{A} and \mathcal{B} have no common point, for every $N \in \mathbb{N}$ and for every complex function f which is defined and sufficiently often differentiable at the multiple nodes of the initial section

$$\mathcal{A}_N = (a_1, \dots, a_N) \tag{8}$$

of \mathcal{A} there is a unique $p \in \mathcal{U}_N$ that satisfies the interpolation conditions

$$\left(\frac{d}{dz}\right)^{\mu_i(a_i)} (p - f)(a_i) = 0, \quad i = 1, \dots, N. \tag{9}$$

Here

$$\mu_i(a) \text{ is the multiplicity of } a \text{ in the sequence } (a_1, \dots, a_{i-1}). \tag{10}$$

We also express the interpolation conditions by saying that u agrees with f at a_1, \dots, a_N counting multiplicities. There is a simple proof due to Walsh [20] reducing it to interpolation by algebraic polynomials. Before repeating this proof we will introduce some notations to simplify formulas to be derived later. We sometimes will assume that the systems \mathcal{A}_N of nodes and \mathcal{B}_N of poles are *consistently ordered*, i.e.,

$$\mathcal{A}_N = (\underbrace{\alpha_1, \dots, \alpha_1}_{m_1}, \underbrace{\alpha_2, \dots, \alpha_2}_{m_2}, \dots, \underbrace{\alpha_p, \dots, \alpha_p}_{m_p}), \tag{11}$$

$$\mathcal{B}_N = (\underbrace{\beta_0, \dots, \beta_0}_{n_0}, \underbrace{\beta_1, \dots, \beta_1}_{n_1}, \dots, \beta_{q-1}, \underbrace{\beta_q, \dots, \beta_q}_{n_q}) \tag{12}$$

corresponding with

$$U_N = \left(1, z, \dots, z^{n_0-1}, \frac{1}{z - \beta_1}, \dots, \frac{1}{(z - \beta_1)^{n_1}}, \dots, \frac{1}{z - \beta_q}, \dots, \frac{1}{(z - \beta_q)^{n_q}}\right), \tag{13}$$

where $\alpha_1, \dots, \alpha_p$ and $\beta_0, \beta_1, \dots, \beta_q$ are pairwise distinct and $m_1 + \dots + m_p = N$, $m_i \geq 0$ and $n_0 + n_1 + \dots + n_q = N$, $n_0 \geq 0$, $n_i \geq 1$ for $i \in \{1, \dots, q\}$, respectively. In most cases, we will assume $\beta_0 = \infty$ to

be in front of the other poles corresponding with (13), in some considerations we assume $\beta_0 = \infty$ at the end of the pole sequence (12),

$$\mathcal{B}_N = (\underbrace{\beta_1, \dots, \beta_1}_{n_1}, \dots, \beta_{q-1}, \underbrace{\beta_q, \dots, \beta_q}_{n_q}, \underbrace{\beta_0, \dots, \beta_0}_{n_0}) \tag{14}$$

corresponding with

$$U_N = \left(\frac{1}{z - \beta_1}, \dots, \frac{1}{(z - \beta_1)^{n_1}}, \dots, \frac{1}{z - \beta_q}, \dots, \frac{1}{(z - \beta_q)^{n_q}}, 1, z, \dots, z^{n_0-1} \right). \tag{15}$$

Notice that p, m_1, \dots, m_p as well as q, n_0, \dots, n_q do depend on N . Of course, there is no loss of generality in assuming that the nodes and poles are ordered consistently. This only means reordering the system U_N keeping it to be an extended complete Čebyšev system on $\mathbb{C} \setminus \{b_1, \dots, b_N\}$ and reordering Eq. (9) according to a permutation of \mathcal{A}_N to get the node system consistently ordered.

Another simplification results from adopting the following notation. If $(\gamma_1, \dots, \gamma_k)$ is a sequence in \mathbb{C} , then

$$\gamma_j^* := \begin{cases} \gamma_j & \text{if } \gamma_j \in \mathbb{C}, \gamma_j \neq 0, \\ 1 & \text{if } \gamma_j = \infty \text{ or } \gamma_j = 0, \end{cases} \tag{16}$$

$$\prod_{j=1}^k \gamma_j^* := \prod_{j=1}^k \gamma_j^*, \tag{17}$$

i.e., the symbol \prod^* means that each factor equal to ∞ or to zero is replaced by a factor 1.

Proof of Proposition 1. Let $A_N(z) = (z - a_1) \cdot \dots \cdot (z - a_N)$ be the *node polynomial* and $B_N = (z - b_1)^* \cdot \dots \cdot (z - b_N)^*$ be the *pole polynomial* associated with the systems \mathcal{A}_N and \mathcal{B}_N , respectively. Let φ be the polynomial of degree $N - 1$ at most that interpolates $B_N f$ at the nodes of \mathcal{A}_N counting multiplicities. Then $p := \varphi/B_N$ satisfies (9). Indeed, $p \in \mathcal{U}_N$ follows from the partial fraction decomposition theorem and, since B_N and A_N are prime, Leibniz' rule combined with an induction argument yields

$$\left(\frac{d}{dz} \right)^{\mu_i(a_i)} (f - p)(a_i) = 0, \quad i = 1, \dots, N \Leftrightarrow \left(\frac{d}{dz} \right)^{\mu_i(a_i)} (B_N f - \varphi)(a_i) = 0, \quad i = 1, \dots, N. \quad \square$$

2. Interpolation by Cauchy–Vandermonde systems

With the node sequence (7) there is naturally associated a sequence

$$\mathcal{L} = (L_1, L_2, \dots), \quad u \mapsto L_i = \left(\frac{d}{dz} \right)^{\mu_i(a_i)} u(a_i) \tag{18}$$

of Hermite-type linear functionals where $\mu_i(a)$ is defined by (10). For interpolation by algebraic polynomials there are well-known classical formulas connected with the names of Lagrange, Newton, Neville and Aitken expressing the interpolant in terms of the nodes and interpolation data

$$w_i = \left(\frac{d}{dz} \right)^{\mu_i(a_i)} f(a_i), \quad i = 1, \dots, N. \tag{19}$$

Since CV-systems in many aspects are close to algebraic polynomials it should be expected that there are similar interpolation formulas for CV-systems. Such formulas are given in the next three subsections.

2.1. Lagrange’s interpolation formula

The basic Lagrange functions ℓ_j ($j = 1, \dots, N$) for the N -dimensional CV-space \mathcal{U}_N are uniquely determined by the conditions of biorthogonality

$$\langle L_i, \ell_j \rangle = \delta_{i,j}, \quad i, j = 1, \dots, N. \tag{20}$$

For certain purposes it is important that we are able to change easily between the one-index enumeration of Hermite functionals (18) corresponding to the one-index enumeration (7) of the nodes and the two-index enumeration

$$\langle L_i, f \rangle = \left(\frac{d}{dz} \right)^\rho f(\alpha_r), \quad r = 1, \dots, p, \quad \rho = 0, \dots, m_r - 1, \tag{21}$$

where we assume that \mathcal{A}_N is consistently ordered as in (11). This is done by the one-to-one mapping $\varphi = \varphi_N$:

$$(r, \rho) \xrightarrow{\varphi} i = \varphi(r, \rho) = m_1 + \dots + m_{r-1} + \rho + 1. \tag{22}$$

Similarly, between the enumeration of the CV functions (2) corresponding to the one-index enumeration (1) of the poles and the two-index enumeration

$$u_j = u_{s,\sigma}, \quad s = 0, \dots, q, \quad \sigma = 1, \dots, n_s, \tag{23}$$

where

$$u_{s,\sigma}(z) = \begin{cases} \frac{1}{(z - b_s)^\sigma} & s = 1, \dots, q, \quad \sigma = 1, \dots, n_s, \\ z^{\sigma-1} & s = 0, \quad \sigma = 1, \dots, n_0 \end{cases} \tag{24}$$

corresponding to the consistently ordered pole system (15), there is the one-to-one mapping $\psi = \psi_N$:

$$(s, \sigma) \xrightarrow{\psi} j = \psi(s, \sigma) = n_1 + \dots + n_{s-1} + \sigma. \tag{25}$$

In order to give a Lagrange-type formula the following notation is needed:

$$B_N(z) = \prod_{j=1}^N (z - b_j) = \prod_{t=1}^q (z - \beta_t)^{n_t},$$

$$\omega_\ell(z) = \prod_{\substack{s=1 \\ s \neq \ell}}^p (z - \alpha_s)^{m_s}, \quad \ell = 1, \dots, p,$$

$$v_{\ell,\lambda}(z) = \frac{1}{\lambda!} (z - \alpha_\ell)^\lambda, \quad \ell = 1, \dots, p, \quad \lambda = 0, \dots, m_\ell - 1,$$

$$P_{\ell,\lambda}(z) = \sum_{i=0}^{m_\ell-\lambda-1} \frac{1}{i!} \left(\frac{d}{dz}\right)^i \left(\frac{B_N}{\omega_\ell}\right) (\alpha_\ell)(z - \alpha_\ell)^i,$$

$$d_\ell^i(\cdot) = \left(\frac{d}{dz}\right)^i (\cdot)_{z=\alpha_\ell}, \quad \ell = 1, \dots, p, \quad i = 0, \dots, m_\ell - 1.$$

Proposition 2. Assume that node system (8) and pole system (5) when consistently ordered are identical with (11) and (14), respectively. Given a function f that is defined on \mathcal{A}_N and sufficiently often differentiable at the multiple nodes, the interpolant $p \in \mathcal{U}_N$ of f at \mathcal{A}_N admits the Lagrange-type representation,

$$p = p \begin{bmatrix} u_1, \dots, u_N \\ a_1, \dots, a_N \end{bmatrix} f = p_1^N f = \sum_{i=1}^N \left(\frac{d}{dz}\right)^{\mu_i(a_i)} f(a_i) \ell_i = \sum_{\ell=1}^p \sum_{\lambda=0}^{m_\ell-1} \left(\frac{d}{dz}\right)^\lambda f(\alpha_\ell) \omega_\ell^\lambda, \tag{26}$$

where the Lagrange-type basis functions are

$$\ell_i(z) = \ell_{\varphi(\ell,\lambda)}(z) = \omega_\ell^\lambda(z) = \frac{\omega_\ell(z)}{B_N(z)} P_{\ell,\lambda}(z) v_{\ell,\lambda}(z). \tag{27}$$

Observe that in case all poles are at infinity formula (26) reduces to the well-known Lagrange–Hermite interpolation formula [2] for interpolation by algebraic polynomials.

The *proof* [12] is simple. One only has to check that the functions $\omega_\ell^\lambda \in \mathcal{U}_N$ are biorthogonal to the functionals d_s^σ which can be verified by repeatedly using the Leibniz’ formula. \square

It is another simple task to find the coefficients $A_{s,\sigma}^{\ell,\lambda}$ of the partial fraction decomposition in

$$\omega_\ell^\lambda = \sum_{s=0}^q \sum_{\sigma=1}^{n_s} A_{s,\sigma}^{\ell,\lambda} u_{s,\sigma},$$

$$A_{s,\sigma}^{\ell,\lambda} = \begin{cases} \frac{D_s^{n_s-\sigma} [\omega_\ell P_{\ell,\lambda} v_{\ell,\lambda}]}{(n_s - \sigma)! \prod_{t=1, t \neq s}^q (\beta_s - \beta_t)^{n_t}}, & s = 1, \dots, q, \quad \sigma = 1, \dots, n_s, \\ \frac{D_0^{n_0-\sigma}}{(n_0 - \sigma)!} \left[\frac{\omega_\ell P_{\ell,\lambda} v_{\ell,\lambda}}{B_N z^{n_0-1}} \right], & s = 0, \quad \sigma = 1, \dots, n_0. \end{cases} \tag{28}$$

Here the differentiation D_s^σ is defined by $D_s^\sigma(\cdot) = (d/dz)^\sigma(\cdot)_{z=\beta_s}$.

By somewhat tedious but elementary calculations it is possible to express the coefficients (28) solely in terms of the nodes and poles [12]. If one knows the coefficients $c_{j,t} = A_{\psi^{-1}(t)}^{\varphi^{-1}(j)}$ of the expansion

$$\ell_j = \sum_{t=1}^N c_{j,t} u_t, \quad j = 1, \dots, N, \tag{29}$$

it is easy to give an explicit formula of the inverse of the *Cauchy–Vandermonde matrix*

$$V := V \begin{pmatrix} u_1, \dots, u_N \\ L_1, \dots, L_N \end{pmatrix} = (\langle L_i, u_j \rangle)_{i=1, \dots, N}^{j=1, \dots, N}. \tag{30}$$

In fact, since for $j = 1, \dots, N$,

$$\ell_j = \frac{1}{\det V} \begin{vmatrix} \langle L_1, u_1 \rangle & \dots & \dots & \dots & \langle L_1, u_N \rangle \\ \vdots & & & & \vdots \\ \langle L_{j-1}, u_1 \rangle & \dots & \dots & \dots & \langle L_{j-1}, u_N \rangle \\ u_1 & \dots & \dots & \dots & u_N \\ \langle L_{j+1}, u_1 \rangle & \dots & \dots & \dots & \langle L_{j+1}, u_N \rangle \\ \vdots & & & & \vdots \\ \langle L_N, u_1 \rangle & \dots & \dots & \dots & \langle L_N, u_N \rangle \end{vmatrix} \tag{31}$$

the adjoint V_{adj} of V equals

$$V_{\text{adj}} = (\det V)C \tag{32}$$

where C has entries $c_{j,t}$ defined by (29). Hence

$$V^{-1} = C^T. \tag{33}$$

It is remarkable [6] that in case of q simple finite poles and a pole at infinity of multiplicity n_0 , $q + n_0 = N$, and N simple nodes the inverse of V can be factorized as

$$V^{-1} = \begin{pmatrix} D_1 & 0 \\ 0 & H(s) \end{pmatrix} V^T D_2, \tag{34}$$

where D_1, D_2 are diagonal matrices of dimensions q and N , respectively, and where $H(s)$ is a triangular Hankel matrix of the form

$$H(s) = \begin{pmatrix} s_1 & s_2 & s_3 & \dots & s_{n_q} \\ s_2 & s_3 & \dots & \cdot & \\ s_3 & \dots & \cdot & & \\ \cdot & \cdot & & & \\ \cdot & & & & \\ s_{n_q} & & & & \end{pmatrix}.$$

2.2. The Neville–Aitken interpolation formula

In [7] a Neville-Algorithm is given which computes the whole triangular field

$$(p_i^k f)_{i=1, \dots, N-k+1}^{k=1, \dots, N}, \quad p_i^k f = p \begin{bmatrix} u_1, \dots, u_k \\ a_i, \dots, a_{i+k-1} \end{bmatrix} f \in \mathcal{U}_k \tag{35}$$

of interpolants recursively where $p_i^k f$ agrees with the function f on $\{a_i, \dots, a_{i+k-1}\}$. In [7] this algorithm was derived from the general Neville–Aitken algorithm [11,3] via explicit formulas for the Cauchy–Vandermonde determinants [17]. In [5] we were going the other way around and have given a different proof of the Neville–Aitken algorithm which is purely algebraic. In this survey we will derive the algorithm by a simple direct argument.

Proposition 3. Let $k \in \mathbb{N}$,

$$\mathcal{A}_{k+1} = (a_1, \dots, a_k, a_{k+1}) = (\underbrace{\alpha_1, \dots, \alpha_1}_{m_1}, \alpha_2, \dots, \alpha_{p-1}, \underbrace{\alpha_p, \dots, \alpha_p}_{m_p}) \in \mathbb{C}^{k+1},$$

with $\alpha_1, \dots, \alpha_p$ pairwise distinct and $m_1 + \dots + m_p = k + 1$, $\mathcal{A}_k = (a_1, \dots, a_k)$, $\mathcal{A}'_k = (a_2, \dots, a_{k+1})$ and $a_1 \neq a_{k+1}$. Let $\mathcal{U}_{k+1} = (u_1, \dots, u_{k+1})$ be a CV-system associated with the pole system $\mathcal{B}_{k+1} = (b_1, \dots, b_{k+1})$. Suppose $\mathcal{A}_{k+1} \cap \mathcal{B}_{k+1} = \emptyset$. Let $p_1 \in \mathcal{U}_k$ interpolate f at \mathcal{A}_k and $p_2 \in \mathcal{U}_k$ interpolate f at \mathcal{A}'_k and let $p_3 \in \mathcal{U}_{k+1}$ interpolate f at \mathcal{A}_{k+1} .

(i) If $b_{k+1} \in \mathbb{C}$ then

$$p_3(z) = \frac{p_1(z)(z - a_{k+1})(b_{k+1} - a_1) - p_2(z)(z - a_1)(b_{k+1} - a_{k+1})}{(a_{k+1} - a_1)(z - b_{k+1})}. \tag{36}$$

(ii) If $b_{k+1} = \infty$ then

$$p_3(z) = \frac{p_1(z)(z - a_{k+1}) - p_2(z)(z - a_1)}{a_1 - a_{k+1}}. \tag{37}$$

Proof. (i) Call the right-hand side of (36) \tilde{p}_3 . It belongs to \mathcal{U}_{k+1} in view of

$$\frac{z - a_{k+1}}{z - b_{k+1}} = 1 + \frac{b_{k+1} - a_{k+1}}{z - b_{k+1}} \quad \text{and} \quad \frac{z - a_1}{z - b_{k+1}} = 1 + \frac{b_{k+1} - a_1}{z - b_{k+1}}$$

by the partial fraction decomposition theorem. Obviously, \tilde{p}_3 interpolates f at \mathcal{A}_{k+1} if all nodes are simple since the weights add to one and each of the unknown values $p_1(a_{k+1})$, $p_2(a_1)$ has factor 0. It is a consequence of Leibniz' rule that this holds true also in case of multiple nodes. In fact,

$$\begin{aligned} & \left(\frac{d}{dz}\right)^\mu \tilde{p}_3|_{z=\alpha_i} \\ &= \frac{b_{k+1} - a_1}{a_{k+1} - a_1} \left(\frac{d}{dz}\right)^\mu \left[p_1(z) \frac{z - a_{k+1}}{z - b_{k+1}} \right]_{z=\alpha_i} - \frac{b_{k+1} - a_{k+1}}{a_{k+1} - a_1} \left(\frac{d}{dz}\right)^\mu \left[p_2(z) \frac{z - a_1}{z - b_{k+1}} \right]_{z=\alpha_i} \\ &= \frac{b_{k+1} - a_1}{a_{k+1} - a_1} \sum_{\lambda=0}^\mu \binom{\mu}{\lambda} \left(\frac{d}{dz}\right)^\lambda p_1(z)|_{z=\alpha_i} \left(\frac{d}{dz}\right)^{\mu-\lambda} \frac{z - a_{k+1}}{z - b_{k+1}}|_{z=\alpha_i} \\ &\quad - \frac{b_{k+1} - a_{k+1}}{a_{k+1} - a_1} \sum_{\lambda=0}^\mu \binom{\mu}{\lambda} \left(\frac{d}{dz}\right)^\lambda p_2(z)|_{z=\alpha_i} \left(\frac{d}{dz}\right)^{\mu-\lambda} \frac{z - a_1}{z - b_{k+1}}|_{z=\alpha_i} \\ &= \frac{b_{k+1} - a_1}{a_{k+1} - a_1} \sum_{\lambda=0}^\mu \binom{\mu}{\lambda} \left(\frac{d}{dz}\right)^\lambda f(z)|_{z=\alpha_i} \left(\frac{d}{dz}\right)^{\mu-\lambda} \frac{z - a_{k+1}}{z - b_{k+1}}|_{z=\alpha_i} \\ &\quad - \frac{b_{k+1} - a_{k+1}}{a_{k+1} - a_1} \sum_{\lambda=0}^\mu \binom{\mu}{\lambda} \left(\frac{d}{dz}\right)^\lambda f(z)|_{z=\alpha_i} \left(\frac{d}{dz}\right)^{\mu-\lambda} \frac{z - a_1}{z - b_{k+1}}|_{z=\alpha_i} \\ &= \left(\frac{d}{dz}\right)^\mu \left[\frac{b_{k+1} - a_1}{a_{k+1} - a_1} f(z) \frac{z - a_{k+1}}{z - b_{k+1}} - \frac{b_{k+1} - a_{k+1}}{a_{k+1} - a_1} f(z) \frac{z - a_1}{z - b_{k+1}} \right]_{z=\alpha_i} \\ &= \left(\frac{d}{dz}\right)^\mu f(z)|_{z=\alpha_i} \end{aligned}$$

since the weights add to one. This is evident for all $i = 1, \dots, p$ and $\mu = 0, \dots, m_p - 1$ except for $i = 1$ and $\mu = m_1 - 1$ or $i = p$ and $\mu = m_p - 1$. If $i = 1$ and $\mu = m_1 - 1$ then the unknown derivative

$(d/dz)^{m_1-1} p_2(z)|_{z=\alpha_1}$ has the factor $(z - a_1)/(z - b_{k+1})|_{z=\alpha_1}$ which vanishes. Similarly, for $i = p$ and $\mu = m_p - 1$ the unknown derivative $(d/dz)^{m_p-1} p_1(z)|_{z=\alpha_p}$ has the factor $(z - a_{k+1})/(z - b_{k+1})|_{z=\alpha_p}$ which vanishes.

(ii) Obviously, the right-hand side of (37) belongs to \mathcal{U}_{k+1} and satisfies the interpolation conditions as is shown by the same argument used in the proof of (i). \square

Remarks.

1. Letting $b_{k+1} \rightarrow \infty$ in (36) gives an alternative proof of (37). Observe that (37) is the classical Neville–Aitken recursion for interpolation by polynomials. It has to be used anytime a pole ∞ is inserted.
2. $p_3(z)$ is a convex combination of $p_1(z)$ and $p_2(z)$ if a_1, a_{k+1}, z, b_{k+1} are real and $a_1 \leq z \leq a_{k+1} < b_{k+1}$ or $b_{k+1} < a_1 \leq z \leq a_{k+1}$.
3. Proposition 2 constitutes an algorithm of arithmetical complexity $\mathcal{O}(N^2)$ to compute the triangular field (35) recursively from initializations $p_i^\ell f \in \mathcal{U}_\ell$ ($\ell \geq 1$) which are generalized Taylor interpolants: $p_i^\ell f$ agrees with f at $(a_i, \dots, a_{i+\ell-1})$ where all nodes are identical $a_i = \dots = a_{i+\ell-1} =: a$. From (26) and (27) immediately

$$p_i^\ell(f) = \sum_{\lambda=0}^{\ell-1} \left(\frac{d}{dz} \right)^\lambda f(a) \omega_1^\lambda \tag{38}$$

with

$$\omega_1^\lambda = \frac{1}{B_\ell(z)} \sum_{\mu=0}^{\ell-\lambda-1} \frac{(d/dz)^\mu B_\ell(a)}{\mu!} (z - a)^{\mu+\lambda} \in \mathcal{U}_\ell \tag{39}$$

are derived.

2.3. *Newton’s formula and the interpolation error*

Given a complex function f which is defined and sufficiently often differentiable at the multiple nodes of system (8) then (9) constitutes a system of linear equations for the coefficients c_j of the generalized polynomial

$$p = pf =: \sum_{j=1}^N c_j u_j \in \mathcal{U}_N, \tag{40}$$

where the coefficient

$$c_j = c_{1,j}^N(f) = \left[\begin{array}{c|c} u_1, \dots, u_N & f \\ \hline a_1, \dots, a_N & j \end{array} \right]$$

will be referred to as the j th *divided difference* of f with respect to the systems U_N and \mathcal{A}_N . In [6,9] for consistently ordered poles which are assumed to be simple if finite and for simple nodes algorithms for solving system (9) recursively are derived whose arithmetical complexity is $\mathcal{O}(N^2)$.

In this section we are going to derive Newton’s formula for the interpolant obtained in [14] and a procedure to compute the divided differences

$$\left[\begin{array}{c|c} u_1, \dots, u_{k+1} & f \\ \hline a_i, \dots, a_{i+k} & k + 1 \end{array} \right]$$

recursively [14], see also [10,16]. For the latter a new short proof is given. This way we will establish an algorithm to compute the interpolant (40) in the general case of multiple nodes and multiple poles in Newton’s form recursively whose arithmetical complexity again is $\mathcal{O}(N^2)$. Later, in Proposition 6 of Section 4, we will derive an algorithm solving the linear system (9) recursively in the general case of multiple poles and multiple nodes avoiding the additional partial fraction decomposition.

Proposition 4. *If $p_1^k f = : \sum_{j=1}^k c_{1,j}^k(f) u_j \in \mathcal{U}_k$ interpolates f at $\mathcal{A}_k = (a_1, \dots, a_k)$ and $p_1^{k+1} f = : \sum_{j=1}^{k+1} c_{1,j}^{k+1}(f) u_j \in \mathcal{U}_{k+1}$ interpolates f at $\mathcal{A}_{k+1} = (a_1, \dots, a_k, a_{k+1})$, then*

$$p_1^{k+1} f = p_1^k f + c_{1,k+1}^{k+1}(f) r_1^k u_{k+1}, \tag{41}$$

where

$$r_1^k u_{k+1}(z) = u_{k+1}(z) - p_1^k u_{k+1}(z) = \frac{A_k(z)}{B_{k+1}(z)} \frac{B_k(b_{k+1})}{A_k(b_{k+1})} \tag{42}$$

with A_k the node polynomial associated with \mathcal{A}_k , $A_k(b_{k+1}) := \prod_{j=1}^k (b_{k+1} - a_j)$ and with B_k, B_{k+1} the pole polynomials associated with the pole systems \mathcal{B}_k and \mathcal{B}_{k+1} , respectively. Furthermore,

$$c_{1,k+1}^{k+1}(f) = \left[\begin{array}{c|c} u_1, \dots, u_{k+1} & f \\ \hline a_1, \dots, a_{k+1} & k+1 \end{array} \right]$$

with

$$\left[\begin{array}{c|c} u_1, \dots, u_{k+1} & f \\ \hline a_1, \dots, a_{k+1} & k+1 \end{array} \right] = \begin{cases} \frac{\left[\begin{array}{c|c} u_1, \dots, u_k & f \\ \hline a_2, \dots, a_{k+1} & k \end{array} \right] - \left[\begin{array}{c|c} u_1, \dots, u_k & f \\ \hline a_1, \dots, a_k & k \end{array} \right]}{\frac{a_{k+1} - a_1}{(a_{k+1} - b_{k+1})^*} \cdot \frac{B_k(b_{k+1})}{A_k(b_{k+1})} \cdot \frac{A'_{k-1}(b_k)}{B_{k-1}(b_k)}}} & \text{if } a_1 \neq a_{k+1}, \\ \det V \left(\begin{array}{c} u_1, \dots, u_{k-1}, f \\ a, \dots, a, a \end{array} \right) / \det V \left(\begin{array}{c} u_1, \dots, u_{k-1}, u_k \\ a, \dots, a, a \end{array} \right) & \end{cases} \tag{43}$$

if in the second case all nodes are identical $a_1 = \dots = a_{k+1} = a$. Here $A'_{k-1}(b_{k+1}) := \prod_{j=2}^k (b_{k+1} - a_j)$. For any $z \in \mathbb{C} \setminus \mathcal{B}_k$

$$r_1^k f(z) = f(z) - p_1^k f(z) = [a_1, \dots, a_k, z] (B_k f) \frac{A_k(z)}{B_k(z)} \tag{44}$$

with

$$[a_1, \dots, a_k, z] (B_k f) = \sum_{i=1}^k [a_1, \dots, a_i] B_k [a_i, \dots, a_k, z] f + [a_1, \dots, a_k, z] B_k f(z) \tag{45}$$

denoting the ordinary divided difference where $[a_1, \dots, a_k, z] B_k = 0$ iff at least one pole is at infinity. Moreover, if $b_{k+1} \in \bar{\mathbb{C}}$ is chosen arbitrarily,

$$r_1^k f(z) = \left[\begin{array}{c|c} u_1, \dots, u_{k+1} & f \\ \hline a_1, \dots, a_k, z & k+1 \end{array} \right] \frac{A_k(z) B_k(b_{k+1})}{B_{k+1}(z) A_k(b_{k+1})}. \tag{46}$$

Proof. Consider linear system (9) for the coefficients of $p_1^{k+1} f$:

$$V \left(\begin{array}{c} u_1, \dots, u_{k+1} \\ L_1, \dots, L_{k+1} \end{array} \right) \left(\begin{array}{c} c_{1,1}^{k+1}(f) \\ \vdots \\ c_{1,k+1}^{k+1}(f) \end{array} \right) = \left(\begin{array}{c} \langle L_1, f \rangle \\ \vdots \\ \langle L_{k+1}, f \rangle \end{array} \right)$$

bordered by the equation

$$\sum_{j=1}^{k+1} c_{1,j}^{k+1}(f)u_j(z) + \xi = 0$$

thus introducing a new unknown $\xi = -p_1^{k+1}f(z)$ where $z \notin \{a_1, \dots, a_{k+1}\}$ is arbitrary. The new system reads

$$\begin{pmatrix} V \begin{pmatrix} u_1, \dots, u_{k+1} \\ L_1, \dots, L_{k+1} \end{pmatrix} & \mathbf{0} \\ \langle L, u_1 \rangle \dots \langle L, u_{k+1} \rangle & 1 \end{pmatrix} \begin{pmatrix} \mathbf{c} \\ \xi \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix}, \tag{47}$$

where $\langle L, u_j \rangle := u_j(z)$ ($j = 1, \dots, k + 1$), $\mathbf{c} = (c_{1,1}^{k+1}(f), \dots, c_{1,k+1}^{k+1}(f))^\top$ and $\mathbf{b} = (\langle L_i, f \rangle)_{i=1, \dots, k+1}$ with $\langle L, f \rangle := 0$. By block elimination of the unknowns c_1, \dots, c_k in the last equation of the bordered system using

$$V \begin{pmatrix} u_1, \dots, u_k \\ L_1, \dots, L_k \end{pmatrix}$$

as pivot we get the equation

$$\alpha_1 c_{1,k+1}^{k+1}(f) + \xi = \beta_1.$$

Here α_1, β_1 are certain Schur complements:

$$\begin{aligned} \alpha_1 &= \det V \begin{pmatrix} u_1, \dots, u_k, u_{k+1} \\ L_1, \dots, L_k, L \end{pmatrix} / \det V \begin{pmatrix} u_1, \dots, u_k \\ L_1, \dots, L_k \end{pmatrix} = \langle L, r_1^k u_{k+1} \rangle \\ &= \langle L, u_{k+1} \rangle - (\langle L, u_1 \rangle, \dots, \langle L, u_k \rangle) V \begin{pmatrix} u_1, \dots, u_k \\ L_1, \dots, L_k \end{pmatrix}^{-1} \begin{pmatrix} \langle L_1, u_{k+1} \rangle \\ \vdots \\ \langle L_k, u_{k+1} \rangle \end{pmatrix}, \end{aligned} \tag{48}$$

similarly,

$$\beta_1 = V \begin{pmatrix} u_1, \dots, u_k, f \\ L_1, \dots, L_k, L \end{pmatrix} / V \begin{pmatrix} u_1, \dots, u_k \\ L_1, \dots, L_k \end{pmatrix} = -p_1^k f(z).$$

Since z is arbitrary this yields Eq. (41). It holds trivially for $z \in \{a_1, \dots, a_k\}$.

The proof of (42) starts from the obvious representation

$$\det V \begin{pmatrix} u_1, \dots, u_k, u_{k+1} \\ L_1, \dots, L_k, L \end{pmatrix} = e \frac{A_k(z)}{B_{k+1}(z)}, \tag{49}$$

where A_k is the node polynomial associated with \mathcal{A}_k and B_{k+1} is the pole polynomial associated with \mathcal{B}_{k+1} and where e must be a constant. To determine e consider the partial fraction decomposition of $A_k(z)/B_{k+1}(z) = \sum_{j=1}^{k+1} d_j u_j(z)$. It is easy to see that in any case

$$d_{k+1} = \frac{A_k(b_{k+1})}{B_k(b_{k+1})}. \tag{50}$$

By comparing coefficients of u_{k+1} on both sides of (49) we find

$$\det V \begin{pmatrix} u_1, \dots, u_k \\ L_1, \dots, L_k \end{pmatrix} = e d_{k+1}. \tag{51}$$

Now (42) follows from (48)–(51).

To prove the remainder formulas (44) and (46) consider the node system $\tilde{\mathcal{A}}_{k+1} := (a_1, \dots, a_k, z)$ with $z \in \mathbb{C} \setminus \mathcal{B}_k$. From Walsh’s proof of Proposition 1 we see that for $z \notin \{a_1, \dots, a_k\}$ the interpolation error is

$$r_1^k f(z) = p_1^{k+1} f(z) - p_1^k f(z) = [a_1, \dots, a_k, z](B_k f) \frac{A_k(z)}{B_k(z)}. \tag{52}$$

If $z \in \{a_1, \dots, a_k\}$ (44) holds trivially. Eq. (45) results by application of Leibniz’ rule for ordinary divided differences. Let $b_{k+1} \in \mathbb{C}$ be arbitrary. By applying (41) to $\tilde{\mathcal{A}}_{k+1}$ with $z \in \mathbb{C} \setminus (\mathcal{B}_k \cup \mathcal{A}_k)$ (46) results. Again, (46) holds trivially, if $z \in \mathcal{A}_k$.

By comparison of (46) and (44) the following relation between ordinary and generalized divided differences obtains

$$\left[\begin{matrix} u_1, \dots, u_{k+1} \\ a_1, \dots, a_k, z \end{matrix} \middle| \begin{matrix} f \\ k+1 \end{matrix} \right] = (z - b_{k+1})^* \frac{A_k(b_{k+1})}{B_k(b_{k+1})} [a_1, \dots, a_k, z](B_k f). \tag{53}$$

Clearly, Eq. (53) holding for all $z \notin \{a_1, \dots, a_k\}$ remains true for arbitrary $z = a_{k+1} \in \mathbb{C} \setminus \mathcal{B}_{k+1}$ by continuity of ordinary divided differences as functions of the nodes showing that the generalized divided differences on the left-hand side share this property. Moreover, using the well-known recurrence relation for ordinary divided differences from (53) with $z = a_{k+1}$ yields

$$\left[\begin{matrix} u_1, \dots, u_{k+1} \\ a_1, \dots, a_{k+1} \end{matrix} \middle| \begin{matrix} f \\ k+1 \end{matrix} \right] = (a_{k+1} - b_{k+1})^* \frac{A_k(b_{k+1})}{B_k(b_{k+1})} \frac{[a_2, \dots, a_{k+1}](B_k \cdot f) - [a_1, \dots, a_k](B_k f)}{a_{k+1} - a_1}. \tag{54}$$

Leibniz’ rule for ordinary divided differences gives

$$\begin{aligned} [a_2, \dots, a_{k+1}](B_k f) &= [a_2, \dots, a_{k+1}]((z - b_k)B_{k-1} f) \\ &= (a_{k+1} - b_k)^* [a_2, \dots, a_{k+1}](B_{k-1} f) + 1[a_2, \dots, a_k](B_{k-1} f), \end{aligned}$$

$$\begin{aligned} [a_1, \dots, a_k](B_k f) &= [a_1, \dots, a_k]((z - b_k)B_{k-1} f) \\ &= (a_1 - b_k)^* [a_1, \dots, a_k](B_{k-1} f) + 1[a_2, \dots, a_k](B_{k-1} f) \end{aligned}$$

and by subtraction

$$\begin{aligned} &\frac{[a_2, \dots, a_{k+1}](B_k f) - [a_1, \dots, a_k](B_k f)}{a_{k+1} - a_1} \\ &= \frac{(a_{k+1} - b_k)^* [a_2, \dots, a_{k+1}](B_{k-1} f) - (a_1 - b_k)^* [a_1, \dots, a_k](B_{k-1} f)}{a_{k+1} - a_1}. \end{aligned}$$

Now (43) follows if the last expression is inserted on the right-hand side of (54). \square

Example. Given $\mathcal{A}_5 = (0, 0, 1, 1, -2)$ and $\mathcal{B}_5 = (\infty, \infty, -1, -1, 2)$ corresponding with $U_5 = (u_1, u_2, u_3, u_4, u_5)$ with

$$u_1(z) = 1, \quad u_2(z) = z, \quad u_3(z) = \frac{1}{z+1}, \quad u_4(z) = \frac{1}{(z+1)^2}, \quad u_5(z) = \frac{1}{z-2}.$$

Given of a function f the interpolation data

$$f(0) = \frac{3}{2}, \quad f'(0) = -2, \quad f(1) = \frac{3}{4}, \quad f'(1) = -\frac{3}{8}, \quad f(-2) = -\frac{9}{8},$$

find $p \in \mathcal{U}_5$ that agrees with f at \mathcal{A}_5 .

According to (43) we easily compute the table of divided differences of f :

z_i	$\begin{bmatrix} u_1 & f \\ \cdot & 1 \end{bmatrix}$	$\begin{bmatrix} u_1 & u_2 & f \\ \cdot & \cdot & 2 \end{bmatrix}$	$\begin{bmatrix} u_1 & u_2 & u_3 & f \\ \cdot & \cdot & \cdot & 3 \end{bmatrix}$	$\begin{bmatrix} u_1 & u_2 & u_3 & u_4 & f \\ \cdot & \cdot & \cdot & \cdot & 4 \end{bmatrix}$
0	$\begin{bmatrix} u_1 & f \\ 0 & 1 \end{bmatrix} = \frac{3}{2}$			
0		$\begin{bmatrix} u_1 & u_2 & f \\ 0 & 0 & 2 \end{bmatrix} = -2$		
1	$\begin{bmatrix} u_1 & f \\ 1 & 1 \end{bmatrix} = \frac{3}{4}$	$\begin{bmatrix} u_1 & u_2 & f \\ 0 & 1 & 2 \end{bmatrix} = -\frac{3}{4}$	$\begin{bmatrix} u_1 & u_2 & u_3 & f \\ 0 & 0 & 1 & 3 \end{bmatrix} = \frac{5}{2}$	
1		$\begin{bmatrix} u_1 & u_2 & f \\ 1 & 1 & 2 \end{bmatrix} = -\frac{3}{8}$	$\begin{bmatrix} u_1 & u_2 & u_3 & f \\ 0 & 0 & 1 & 3 \end{bmatrix} = \frac{3}{2}$	$\begin{bmatrix} u_1 & u_2 & u_3 & u_4 & f \\ 0 & 0 & 1 & 1 & 4 \end{bmatrix} = 2$
-2	$\begin{bmatrix} u_1 & f \\ -2 & 1 \end{bmatrix} = -\frac{9}{4}$	$\begin{bmatrix} u_1 & u_2 & f \\ 1 & -2 & 2 \end{bmatrix} = 1$	$\begin{bmatrix} u_1 & u_2 & u_3 & f \\ 1 & 1 & -2 & 3 \end{bmatrix} = \frac{11}{6}$	$\begin{bmatrix} u_1 & u_2 & u_3 & u_4 & f \\ 0 & 1 & 1 & -2 & 4 \end{bmatrix} = -\frac{1}{6}$

$$\begin{bmatrix} u_1 & u_2 & u_3 & u_4 & u_5 & f \\ 0 & 0 & 1 & 1 & -2 & 5 \end{bmatrix} = \frac{13}{27}.$$

From Newton’s formula (41) we get the interpolant in Newton’s form

$$p(z) = p_1^5 f(z) = \frac{3}{2} - 2z + \frac{5}{2} \frac{z^2}{z+1} + 2 \frac{-z^2(z-1)}{2(z+1)^2} + \frac{13}{27} \frac{9}{4} \frac{z^2(z-1)^2}{(z+1)^2(z-2)},$$

which, by additional partial fraction decompositions, equals

$$p_1^5 f(z) = -\frac{1}{6} + \frac{7}{12}z + \frac{73}{54} \frac{1}{z+1} + \frac{5}{9} \frac{1}{(z+1)^2} + \frac{13}{27} \frac{1}{z-2}.$$

In Section 4 we will present an alternative method computing the interpolant avoiding the additional partial fraction decompositions.

3. Cauchy–Vandermonde determinants

In this section we give a new short proof of the explicite formula of the Cauchy–Vandermonde determinant [17,7,15] in terms of the nodes and poles. It will be derived as a simple consequence of Proposition 4.

Proposition 5. *For consistently ordered node and pole systems as in (11) and (12) that have no common points*

$$\det V \begin{pmatrix} u_1, \dots, u_N \\ L_1, \dots, L_N \end{pmatrix} = \text{mult}(\mathcal{A}_N) \frac{\prod_{\substack{k,j=1 \\ k>j}}^N *(a_k - a_j) \prod_{\substack{k,j=1 \\ k \geq j}}^N *(a_k - b_j)}{\prod_{\substack{k,j=1 \\ k>j}}^N *(b_k - b_j) \prod_{\substack{k,j=1 \\ k>j}}^N *(b_k - a_j)} \tag{55}$$

with

$$\text{mult}(\mathcal{A}_N) = \prod_{k=1}^N \mu_k(a_k)! \tag{56}$$

where $\mu_k(a)$ is defined by (10) and use is made of notations (16) and (17).

Proof. From (48) and (42) for $k + 1 = N$ we get

$$\begin{aligned} r_1^{N-1} u_N(z) &= \frac{\det V \begin{pmatrix} u_1, \dots, u_{N-1}, u_N \\ L_1, \dots, L_{N-1}, L \end{pmatrix}}{\det V \begin{pmatrix} u_1, \dots, u_{N-1} \\ L_1, \dots, L_{N-1} \end{pmatrix}} \\ &= \frac{(z - a_1) \cdot \dots \cdot (z - a_{N-1})}{(z - b_1)^* \cdot \dots \cdot (z - b_{N-1})^*} \frac{(b_N - b_1)^* \cdot \dots \cdot (b_N - b_{N-1})^*}{(b_N - a_1)^* \cdot \dots \cdot (b_N - a_{N-1})^*}. \end{aligned}$$

As a consequence,

$$\det V \begin{pmatrix} u_1, \dots, u_{N-1}, u_N \\ L_1, \dots, L_{N-1}, L_N \end{pmatrix} = \det V \begin{pmatrix} u_1, \dots, u_{N-1} \\ L_1, \dots, L_{N-1} \end{pmatrix} \left(\frac{d}{dz} \right)^{\mu_N(a_N)} r_1^{N-1} u_N(z) \Big|_{z=a_N}.$$

By Leibniz' rule

$$\left(\frac{d}{dz} \right)^{\mu_N(a_N)} \frac{(z - a_1) \cdot \dots \cdot (z - a_{N-1})}{(z - b_1)^* \cdot \dots \cdot (z - b_{N-1})^* (z - b_N)^*} \Big|_{z=a_N} = \mu_N(a_N)! \frac{\prod_{j=1}^{N-1} (a_N - a_j)^*}{\prod_{j=1}^N (a_N - b_j)^*}.$$

Hence, we have got a recursion for the determinants considered. Since $\det V \begin{pmatrix} u_1 \\ a_1 \end{pmatrix} = \mu_1(a_1)! \cdot 1 / (a_1 - b_1)^*$ an induction argument proves (55). \square

4. Solution of linear CV-systems

In this section we will present a new method solving the system of linear equations (9) recursively where no additional partial fraction decomposition is needed. Its proof is based upon Proposition 3.

Proposition 6. Let $k \in \mathbb{N}$ and let the CV-systems (u_1, \dots, u_k) and $(u_1, \dots, u_k, u_{k+1})$ correspond to the pole systems

$$\mathcal{B}_k = (b_1, \dots, b_k) = (\underbrace{\beta_0, \dots, \beta_0}_{n_0}, \underbrace{\beta_1, \dots, \beta_1}_{n_1}, \dots, \underbrace{\beta_q, \dots, \beta_q}_{n_q})$$

and $\mathcal{B}_{k+1} = (b_1, \dots, b_k, b_{k+1})$, respectively, where it is assumed that \mathcal{B}_k is consistently ordered with $\beta_0 = \infty, \beta_1, \dots, \beta_q \in \mathbb{C}$ pairwise distinct and $n_0 + n_1 + \dots + n_q = k$. We set for $r = 0, \dots, q$,

$$j_r := n_0 + \dots + n_r.$$

Let $\mathcal{A}_k = (a_1, \dots, a_k) \in \mathbb{C}^k$ and $\mathcal{A}_{k+1} = (a_1, \dots, a_k, a_{k+1}) \in \mathbb{C}^{k+1}$ be arbitrary node systems with

$$\alpha_2 := a_{k+1} \neq a_1 =: \alpha_1.$$

By \mathcal{A}'_k we denote the node system $\mathcal{A}'_k = (a_2, \dots, a_{k+1})$. Given a function f defined and sufficiently often differentiable at the multiple nodes of \mathcal{A}_{k+1} . Let

$$\begin{aligned}
 p_1^k f &=: \sum_{j=1}^k c_{1,j}^k(f) u_j \in \mathcal{U}_k && \text{interpolate } f \text{ at } \mathcal{A}_k, \\
 p_2^k f &=: \sum_{j=1}^k c_{2,j}^k(f) u_j \in \mathcal{U}_k && \text{interpolate } f \text{ at } \mathcal{A}'_k, \text{ and} \\
 p_1^{k+1} f &=: \sum_{j=1}^{k+1} c_{1,j}^{k+1}(f) u_j \in \mathcal{U}_{k+1} && \text{interpolate } f \text{ at } \mathcal{A}_{k+1}.
 \end{aligned}$$

For simplicity, the argument f of the divided differences in the following formulas will be dropped.

(i) If $\beta := b_{k+1} \in \mathbb{C} \setminus \{b_1, \dots, b_k\}$ corresponding to $u_{k+1}(z) = 1/(z - \beta)$ then

$$c_{1,j}^{k+1} = \frac{c_{1,j}^k(\beta - \alpha_1) - c_{2,j}^k(\beta - \alpha_2)}{\alpha_2 - \alpha_1} + \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \sum_{\lambda=j+1}^{j_0} (c_{1,\lambda}^k - c_{2,\lambda}^k) \beta^{\lambda-j-1}, \quad j = 1, \dots, j_0, \tag{57}$$

$$\begin{aligned}
 c_{1,j}^{k+1} &= \frac{c_{1,j}^k(\beta - \alpha_1)(\alpha_2 - b_j) - c_{2,j}^k(\beta - \alpha_2)(\alpha_1 - b_j)}{(\alpha_2 - \alpha_1)(\beta - b_j)} \\
 &\quad - \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \sum_{\lambda=j+1}^{j_{r+1}} \frac{c_{1,\lambda}^k - c_{2,\lambda}^k}{(\beta - b_j)^{\lambda-j+1}} \quad j_r < j \leq j_{r+1}; \quad r = 0, \dots, q - 1, \tag{58}
 \end{aligned}$$

$$c_{1,k+1}^{k+1} = \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \left(\sum_{\lambda=1}^{j_0} (c_{1,\lambda}^k - c_{2,\lambda}^k) \beta^{\lambda-1} + \sum_{r=0}^{q-1} \sum_{\lambda=j_r+1}^{j_{r+1}} \frac{c_{1,\lambda}^k - c_{2,\lambda}^k}{(\beta - b_\lambda)^{\lambda-j_r}} \right). \tag{59}$$

(ii) If $\beta := b_{k+1} = \beta_i \in \mathbb{C}$ corresponding with $u_{k+1}(z) = 1/(z - \beta_i)^{n_i+1}$ then

$$c_{1,j}^{k+1} = \frac{c_{1,j}^k(\beta - \alpha_1) - c_{2,j}^k(\beta - \alpha_2)}{\alpha_2 - \alpha_1} + \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \sum_{\lambda=j+1}^{j_0} (c_{1,\lambda}^k - c_{2,\lambda}^k) \beta^{\lambda-j-1}, \quad j = 1, \dots, j_0, \tag{60}$$

$$\begin{aligned}
 c_{1,j}^{k+1} &= \frac{c_{1,j}^k(\beta - \alpha_1)(\alpha_2 - b_j) - c_{2,j}^k(\beta - \alpha_2)(\alpha_1 - b_j)}{(\alpha_2 - \alpha_1)(\beta - b_j)} \\
 &\quad + \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \sum_{\lambda=j+1}^{j_{r+1}} \frac{c_{1,\lambda}^k - c_{2,\lambda}^k}{(\beta - b_j)^{\lambda-j+1}}, \quad j_r < j \leq j_{r+1}, \quad r = 0, \dots, i - 2, i, i + 1, \dots, q - 1, \tag{61}
 \end{aligned}$$

$$\begin{aligned}
 c_{1,j_{i-1}+1}^{k+1} &= \frac{c_{1,j_{i-1}+1}^k(\beta - \alpha_1) - c_{2,j_{i-1}+1}^k(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \\
 &\quad + \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \left[\sum_{\lambda=1}^{j_0} (c_{1,\lambda}^k - c_{2,\lambda}^k) \beta^{\lambda-1} + \sum_{\substack{r=0 \\ r \neq i-1}}^{q-1} \sum_{\lambda=j_r+1}^{j_{r+1}} \frac{c_{1,\lambda}^k - c_{2,\lambda}^k}{(\beta - b_\lambda)^{\lambda-j_r}} \right], \tag{62}
 \end{aligned}$$

$$c_{1,j}^{k+1} = \frac{c_{1,j}^k(\beta - \alpha_1) - c_{2,j}^k(\beta - \alpha_2)}{\alpha_2 - \alpha_1} + \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} (c_{1,j-1}^k - c_{2,j-1}^k), \quad j = j_{i-1} + 2, \dots, j_i, \tag{63}$$

$$c_{1,k+1}^{k+1} = \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} (c_{1,j_i}^k - c_{2,j_i}^k). \tag{64}$$

(iii) If $\beta := b_{k+1} = \infty$ corresponding with $u_{k+1}(z) = z^{n_0}$ then

$$c_{1,1}^{k+1} = \frac{c_{1,1}^k \alpha_2 - c_{2,1}^k \alpha_1 - \sum_{\lambda=0}^{q-1} (c_{1,j_{\lambda+1}}^k - c_{2,j_{\lambda+1}}^k)}{\alpha_2 - \alpha_1}, \tag{65}$$

$$c_{1,j}^{k+1} = \frac{c_{1,j}^k \alpha_2 - c_{2,j}^k \alpha_1 - (c_{1,j-1}^k - c_{2,j-1}^k)}{\alpha_2 - \alpha_1}, \quad j = 2, \dots, j_0, \tag{66}$$

$$c_{1,j}^{k+1} = \frac{c_{1,j}^k \alpha_2 - c_{2,j}^k \alpha_1 - (c_{1,j}^k - c_{2,j}^k) b_j - (c_{1,j+1}^k - c_{2,j+1}^k)}{\alpha_2 - \alpha_1}, \quad j_0 < j < k, \quad j \neq j_1, j_2, \dots, j_q, \tag{67}$$

$$c_{1,j}^{k+1} = \frac{c_{1,j}^k \alpha_2 - c_{2,j}^k \alpha_1 - (c_{1,j}^k - c_{2,j}^k) b_j}{\alpha_2 - \alpha_1}, \quad j = j_i, \quad i = 1, \dots, q, \tag{68}$$

$$c_{1,k+1}^{k+1} = -\frac{c_{1,j_0}^k - c_{2,j_0}^k}{\alpha_2 - \alpha_1}. \tag{69}$$

Proof. According to (36) if $\beta := b_{k+1} \in \mathbb{C}$ we have

$$\begin{aligned} p_1^{k+1} &= \sum_{j=1}^{k+1} c_{1,j}^{k+1} u_j \\ &= \left(\sum_{j=1}^k c_{1,j}^k u_j \right) \left(1 + \frac{\beta - \alpha_2}{z - \beta} \right) \frac{\beta - \alpha_1}{\alpha_2 - \alpha_1} - \left(\sum_{j=1}^k c_{2,j}^k u_j \right) \left(1 + \frac{\beta - \alpha_1}{z - \beta} \right) \frac{\beta - \alpha_2}{\alpha_2 - \alpha_1} \\ &= \frac{1}{\alpha_2 - \alpha_1} \sum_{j=1}^k (c_{1,j}^k(\beta - \alpha_1) - c_{2,j}^k(\beta - \alpha_2)) u_j \\ &\quad + \frac{(\beta - \alpha_1)(\beta - \alpha_2)}{\alpha_2 - \alpha_1} \sum_{j=1}^k (c_{1,j}^k - c_{2,j}^k) u_j \frac{1}{z - \beta}. \end{aligned} \tag{70}$$

If $\beta = \infty$ according to (37) we have

$$\begin{aligned} p_1^{k+1} &= \sum_{j=1}^{k+1} c_{1,j}^{k+1} u_j = \frac{\sum_{j=1}^k c_{1,j}^k u_j (z - \alpha_2) - \sum_{j=1}^k c_{2,j}^k u_j (z - \alpha_1)}{\alpha_1 - \alpha_2} \\ &= \frac{\sum_{j=1}^k (c_{1,j}^k \alpha_2 - c_{2,j}^k \alpha_1) u_j - \sum_{j=1}^k (c_{1,j}^k - c_{2,j}^k) u_j z}{\alpha_2 - \alpha_1}. \end{aligned} \tag{71}$$

Now by partial fraction decomposition

$$z^v \frac{1}{z - \beta} = \sum_{\lambda=0}^{v-1} \beta^{v-\lambda-1} z^\lambda + \beta^v \frac{1}{z - \beta}, \tag{72}$$

$$\frac{1}{(z - b)^{v+1}} \frac{1}{z - \beta} = \sum_{\lambda=0}^v \frac{-1}{(\beta - b)^{\lambda+1}} \frac{1}{(z - b)^{v+1-\lambda}} + \frac{1}{(\beta - b)^{v+1}} \frac{1}{z - \beta}, \tag{73}$$

$$\frac{1}{(z - b)^{v+1}} z = \frac{z - b + b}{(z - b)^{v+1}} = \frac{1}{(z - b)^v} + b \frac{1}{(z - b)^{v+1}}. \tag{74}$$

Eq. (73) is readily verified by multiplying both sides by $(z - b)^{v+1}(z - \beta)$ and making use of the finite geometric series. Eq. (72) follows from

$$\begin{aligned} z^v \frac{1}{z - \beta} &= \frac{(z - \beta + \beta)^v}{z - \beta} = \sum_{\mu=0}^v \binom{v}{\mu} \beta^{v-\mu} (z - \beta)^{\mu-1} \\ &= \frac{\beta^v}{z - \beta} + \sum_{\mu=1}^v \binom{v}{\mu} \beta^{v-\mu} \sum_{\lambda=0}^{\mu-1} \binom{\mu-1}{\lambda} z^\lambda (-\beta)^{\mu-\lambda-1}. \end{aligned}$$

Here the second sum can be extended over $\lambda = 0, \dots, v - 1$ since the binomial coefficients $\binom{\mu-1}{\lambda}$ vanish for the extra summands. By interchanging the two summations we obtain

$$z^v \frac{1}{z - \beta} = \frac{\beta^v}{z - \beta} + \sum_{\lambda=0}^{v-1} z^\lambda \beta^{v-\lambda-1} (-1)^{\lambda-1} \sum_{\mu=1}^v \binom{v}{\mu} \binom{\mu-1}{\lambda} (-1)^\mu.$$

The second sum equals

$$(-1)^v \sum_{\mu=0}^v \binom{v}{\mu} \binom{\mu-1}{\lambda} (-1)^{v-\mu} + (-1)^{\lambda+1} = (-1)^{\lambda+1}$$

since the sum in the last equation is the forward difference $\Delta_1^v f(0) = f^{(v)}(\xi) = 0$, where

$$f(x) = \binom{x-1}{\lambda} = \frac{(x-1)(x-2)\cdots(x-\lambda)}{\lambda!}$$

is a polynomial of degree λ and $\lambda \leq v - 1 < v$.

Let now $v_j := v_j(b_j)$ denote the multiplicity of b_j in (b_1, \dots, b_{j-1}) . Consider case (i): $\beta = b_{k+1} \in \mathbb{C}$, $\beta \notin \{b_1, \dots, b_k\}$. Then from (72) and (73) (for simplicity we drop the argument z)

$$u_j \frac{1}{z - \beta} = \sum_{\lambda=0}^{j-2} \beta^\lambda u_{j-1-\lambda} + \beta^{j-1} u_{k+1}, \quad 1 \leq j \leq j_0, \tag{75}$$

$$u_j \frac{1}{z - \beta} = \sum_{\lambda=0}^v \frac{-1}{(\beta - b_j)^{\lambda+1}} u_{j-\lambda} + \frac{1}{(\beta - b_j)^{v+1}} u_{k+1}, \quad j_0 < j \leq k. \tag{76}$$

In case (ii): $\beta = b_{k+1} = \beta_i \in \mathbb{C}$, from (72) and (73)

$$u_j \frac{1}{z - \beta} = \sum_{\lambda=0}^{j-2} \beta^\lambda u_{j-1-\lambda} + \beta^{j-1} u_{j-1+1}, \quad 1 \leq j \leq j_0 \tag{77}$$

$$u_j \frac{1}{z - \beta} = \sum_{\lambda=0}^v \frac{-1}{(\beta - b_j)^{\lambda+1}} u_{j-\lambda} + \frac{1}{(\beta - b_j)^{v+1}} u_{j-1+1}, \quad j_0 < j \leq j_{i-1} \text{ or } j_i < j \leq k, \tag{78}$$

$$u_j \frac{1}{z - \beta} = u_{j+1}, \quad j_{i-1} < j < j_i, \tag{79}$$

$$u_j \frac{1}{z - \beta} = u_{k+1}, \quad j = j_i. \tag{80}$$

In case (iii): $\beta = b_{k+1} = \infty$ we have

$$u_j z = u_{j+1}, \quad j = 1, \dots, j_0 - 1, \tag{81}$$

$$u_j z = z^{n_0} = u_{k+1}, \quad j = j_0, \tag{82}$$

$$u_j z = u_1 + b_j u_j, \quad j = j_i + 1, i = 0, \dots, q - 1, \tag{83}$$

$$u_j z = u_{j-1} + b_j u_j \quad j_0 + 1 < j \leq k, j \neq j_i + 1, i = 0, \dots, q - 1. \tag{84}$$

Eqs. (81) and (82) are obvious and (83) and (84) follow from (74). The rest of the proof consists in comparing coefficients. \square

Remark. (i) The arithmetical complexity for computing $(c_{1,j}^{k+1})_{j=1,\dots,k+1}$ from $(c_{1,j}^k)_{j=1,\dots,k}$ and $(c_{2,j}^k)_{j=1,\dots,k}$ according to (57)–(64) in cases (i) or (ii) is $\mathcal{O}(k + 1 + \sum_{r=0}^q (n_r - 1)^2)$ and $\mathcal{O}(k + 1)$ in case (iii).

(ii) It should be noticed that the first term in (58) resp. (61) is the recursion (36) with p_1, p_2 replaced by $c_{1,j}^k, c_{2,j}^k$ and with $z = b_j$. Similarly, the first term in (57), (60), (62) and (63) is recursion (37) with p_1, p_2 replaced by $c_{1,j}^k, c_{2,j}^k$ and with $z = b_j$.

Consider once more the *example* given in Section 2.3. According to Proposition 5 we compute the triangular field of solutions

$$p_i^k = p \left[\begin{matrix} u_1, \dots, u_k \\ a_i, \dots, a_{i+k} \end{matrix} \right] =: \sum_{j=1}^k c_{i,j}^k \cdot u_j, \quad k = 1, \dots, 5, \quad i = 1, \dots, 6 - k.$$

The initializations which are certain generalized Taylor polynomials of f are computed according to Proposition 4, or alternatively, according to (38) and (39).

a_i	$p \begin{bmatrix} u_1 \\ \cdot \end{bmatrix}$	$p \begin{bmatrix} u_1 & u_2 \\ \cdot & \cdot \end{bmatrix}$	$p \begin{bmatrix} u_1 & u_2 & u_3 \\ \cdot & \cdot & \cdot \end{bmatrix}$
0	$p \begin{bmatrix} u_1 \\ 0 \end{bmatrix} = \frac{3}{2} \cdot u_1$		
0		$p \begin{bmatrix} u_1 & u_2 \\ 0 & 0 \end{bmatrix} = \frac{3}{2} - 2 \cdot z$	
1	$p \begin{bmatrix} u_1 \\ 1 \end{bmatrix} = \frac{3}{4} \cdot u_1$	$p \begin{bmatrix} u_1 & u_2 \\ 0 & 1 \end{bmatrix} = \frac{3}{2} - \frac{3}{4} \cdot z$	$p \begin{bmatrix} u_1 & u_2 & u_3 \\ 0 & 0 & 1 \end{bmatrix} = -2 + \frac{1}{2} \cdot z + \frac{5}{2} \frac{1}{z+1}$
1		$p \begin{bmatrix} u_1 & u_2 \\ 0 & 1 \end{bmatrix} = \frac{9}{8} - \frac{3}{8} \cdot z$	$p \begin{bmatrix} u_1 & u_2 & u_3 \\ 0 & 1 & 1 \end{bmatrix} = \frac{3}{2} \frac{1}{z+1}$
-2	$p \begin{bmatrix} u_1 \\ -2 \end{bmatrix} = -\frac{9}{8} \cdot u_1$	$p \begin{bmatrix} u_1 & u_2 \\ 1 & -2 \end{bmatrix} = -\frac{1}{4} + z$	$p \begin{bmatrix} u_1 & u_2 & u_3 \\ 1 & 1 & -2 \end{bmatrix} = -\frac{1}{4} + \frac{1}{12} \cdot z + \frac{11}{6} \frac{1}{z+1}$

$$p \begin{bmatrix} u_1 & u_2 & u_3 & u_4 \\ 0 & 0 & 1 & 1 \end{bmatrix} = 2 - \frac{1}{2}z - \frac{5}{2} \frac{1}{z+1} + 2 \frac{1}{(z+1)^2},$$

$$p \begin{bmatrix} u_1 & u_2 & u_3 & u_4 \\ 0 & 1 & 1 & -2 \end{bmatrix} = -\frac{1}{6} + \frac{1}{24}z + \frac{11}{6} \frac{1}{z+1} - \frac{1}{6} \frac{1}{(z+1)^2},$$

$$p \begin{bmatrix} u_1 & u_2 & u_3 & u_4 & u_5 \\ 0 & 0 & 1 & 1 & -2 \end{bmatrix} = -\frac{1}{6} + \frac{7}{12}z + \frac{73}{54} \frac{1}{z+1} + \frac{5}{9} \frac{1}{(z+1)^2} + \frac{13}{27} \frac{1}{z-2}.$$

For a theory of convergence of rational interpolants with prescribed poles to analytic functions as $N \rightarrow \infty$ confer [1].

5. Applications

CV-systems have been used to construct rational B-splines with prescribed poles. A. Gresbrand [8] has found a recursion fomula for such splines that reduces to de Boor’s recursion when all poles are at infinity. Given a weakly increasing sequence $t = (t_j)_{j=0}^{m+1}$ of knots in $[a, b]$ where $t_0 = a$ and $t_{m+1} = b$ are simple knots and $t_i < t_{i+n-1}$ for all i . The extended knot sequence is $t_{\text{ext}} = (t_j)_{j=-n+1}^{m+n}$ where a and b are repeated precisely n times each. Given a pole sequence $(b_1, \dots, b_n) \in \mathbb{R} \setminus [a, b]$ that is consistently ordered with $b_1 = \infty$, then for $j = 0, \dots, m$ define

$$B_0^1 := \chi_{[t_0, t_1]} \quad \text{and} \quad B_j^1 := \chi_{(t_j, t_{j+1})}$$

with χ_S denoting the characteristic function of a set S and for $k = 2, \dots, n$ and for $j = -k + 2, \dots, m$ define

$$\lambda_j^k(x) := \frac{x - t_j}{t_{j+k-1} - t_j} \frac{1}{(k-1)(x - b_k)^*} \frac{\text{perm}(t_{j+i} - b_{\ell+1})_{i=1, \dots, k-1}^{\ell=1, \dots, k-1}}{\text{perm}(t_{j+i} - b_{\ell+1})_{i=1, \dots, k-2}^{\ell=1, \dots, k-2}},$$

$$\mu_j^k(x) := \frac{t_{j+k} - 1 - x}{t_{j+k-1} - t_j} \frac{1}{(k-1)(x - b_k)^*} \frac{\text{perm}(t_{j+i-1} - b_{\ell+1})_{i=1, \dots, k-1}^{\ell=1, \dots, k-1}}{\text{perm}(t_{j+i} - b_{\ell+1})_{i=1, \dots, k-2}^{\ell=1, \dots, k-2}},$$

where the permanent of a matrix $A = (a_{i,j}) \in \mathbb{K}^{n \times n}$ is defined as

$$\text{perm } A = \sum_{\sigma \in S_n} \prod_{i=1}^n a_{i, \sigma(i)}.$$

Here S_n denotes the symmetric group of all permutations of order n . Then for $k = 2, \dots, n$ and $j = -k + 1, \dots, m$

$$B_j^k(x) := \lambda_j^k(x) B_j^{k-1}(x) + \mu_{j+1}^k(x) B_{j+1}^{k-1}(x) \tag{85}$$

are rational B-splines of order k with prescribed poles (b_1, \dots, b_k) , i.e., when restricted to any knot interval then B_j^k belongs to the CV-space \mathcal{U}_k . Gresbrand [8] has proved that

$$B_j^k(x) = \frac{\text{perm}(t_{j+i} - b_{\ell+1})_{i=1, \dots, k-1}^{\ell=1, \dots, k-1}}{(k-1)! B_k(x)} N_j^k(x), \tag{86}$$

where B_k is the pole polynomial associated with the pole system (b_1, \dots, b_k) and $N_j^k(x) = (t_{j+k} - t_j)[t_j, \dots, t_{j+k}] (\cdot - x)_+^{k-1}$ is the ordinary polynomial B-spline function of order k with knots t_j, \dots, t_{j+k} .

The rational B-splines with prescribed poles (84) share many properties with the de Boor B-splines [8]:

1. They can be computed recursively by a de Boor like algorithm, see (83).
2. $\text{supp } B_j^k = \text{supp } N_j^k = [t_j, t_{j+k}]$.
3. B_j^k has precisely the same smoothness as N_j^k iff all poles are chosen in the exterior of $[a, b]$.
4. B_j^k is nonnegative.
5. The B_j^k form a partition of unity.
6. There are knot insertion algorithms.
7. There is a simple connection with NURBS.

The prescribed poles can serve as additional shape-controlling parameters. Given a knot sequence t and a controll polygon corresponding to t_{ext} by suitably choosing the poles “corners” of the B-spline curve can be generated which are more or less sharp while maintaining the smoothness properties controlled by the knot sequence. The splines (84) are an example of Čebyševian splines which when restricted to any knot interval belong to the same CV-space \mathcal{U}_k . In other words for each knot interval the spline curve has the same poles outside of $[a, b]$. Clearly, one can consider also the more general case where in each knot interval $(t_i, t_{i+1}]$ individually for the spline curve poles are prescribed outside $[t_i, t_{i+1}]$. Not surprisingly, then the computation is more laborous, but we expect also in the general case existence of a recursive procedure [4].

We conclude with mentioning another application. Recently, interpolants from CV-spaces have been proved useful for approximation of transfer functions of infinite-dimensional dynamical systems [19].

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The E -algorithm and the Ford–Sidi algorithm

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Abstract

The E -algorithm and the Ford–Sidi algorithm are two general extrapolation algorithms. It is proved that the E -algorithm and the Ford–Sidi algorithm are mathematically (although not operationally) equivalent. A slightly more economical algorithm is given. Operation counts are discussed. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Extrapolation method; Acceleration of convergence; E -algorithm; Ford–Sidi algorithm

1. Introduction

Let (s_n) be a sequence and $(g_j(n))$, $j = 1, 2, \dots$, be known auxiliary sequences. Suppose that there exist unknown constants (c_j) , $j = 1, \dots, k$, such that

$$s_{n+i} = T_k^{(n)} + \sum_{j=1}^k c_j g_j(n+i), \quad i = 0, \dots, k. \quad (1)$$

If the system of linear equations (1) is nonsingular, then by Cramer's rule $T_k^{(n)}$ can be expressed as the ratio of two determinants

$$T_k^{(n)} = \frac{\begin{vmatrix} s_n & \cdots & s_{n+k} \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}. \quad (2)$$

Many known sequence transformations which are used to accelerate the convergence are of the form $(s_n) \mapsto (T_k^{(n)})$. (For a review, see [2].) Two famous recursive algorithms are known to compute $T_k^{(n)}$. One is the E -algorithm proposed by Schneider [6], Håvie [5] and Brezinski [1], independently.

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Schneider and Håvie derived it using Gaussian elimination while Brezinski using Sylvester’s determinantal identity. The other is the Ford–Sidi algorithm [4], which requires a smaller number of arithmetic operations than the E -algorithm. Ford and Sidi derived their algorithm using Sylvester’s identity.

Ford and Sidi [4] mentioned the main difference of the recursion of the E -algorithm and that of the Ford–Sidi algorithm. Brezinski and Redivo Zaglia [3] derived the E -algorithm and the Ford–Sidi algorithm using annihilation difference operators and gave the relations between the two algorithms.

In this paper we show that the E -algorithm and the Ford–Sidi algorithm are mathematically equivalent in the following sense: two algorithms are computing the same quantities but in a different way, and the recurrence relations of the E -algorithm can be derived from those of the Ford–Sidi algorithm, and vice versa.

In Section 2 we review the recurrence relations and the number of operation counts of the two algorithms. In Section 3 we show that the two algorithms are mathematically equivalent. In Section 4 we give an efficient implementation for the Ford–Sidi algorithm. This implementation is slightly more economical than the original implementation for the Ford–Sidi algorithm.

2. The E -algorithm and the Ford–Sidi algorithm — review

Throughout this paper let $s = (s_n)$ be any sequence to be transformed and $g_j = (g_j(n))$, $j = 1, 2, \dots$, be any auxiliary sequences. We denote 1 by the constant sequence with $1_n = 1$, for $n = 0, 1, \dots$. Assume that all denominators are nonzero.

2.1. The E -algorithm

The E -algorithm is defined as follows. For $n = 0, 1, \dots$, the quantities $E_k^{(n)}$ and $g_{k,j}^{(n)}$ are defined by

$$E_0^{(n)} = s_n,$$

$$g_{0,j}^{(n)} = g_j(n), \quad j = 1, 2, \dots,$$

$$E_k^{(n)} = \frac{E_{k-1}^{(n)} g_{k-1,k}^{(n+1)} - E_{k-1}^{(n+1)} g_{k-1,k}^{(n)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}}, \quad k = 1, 2, \dots, \tag{3}$$

$$g_{k,j}^{(n)} = \frac{g_{k-1,j}^{(n)} g_{k-1,k}^{(n+1)} - g_{k-1,j}^{(n+1)} g_{k-1,k}^{(n)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}}, \quad k = 1, 2, \dots; \quad j = k + 1, \dots \tag{4}$$

The recurrence relations (3) and (4) are called the main rule and the auxiliary rule of the E -algorithm, respectively. Brezinski [1] proved the following theorem using Sylvester’s determinantal identity.

Theorem 1. For $n = 0, 1, \dots$, and $k = 1, 2, \dots$, $E_k^{(n)}$ and $g_{k,j}^{(n)}$ are represented as

$$E_k^{(n)} = \left| \begin{array}{ccc} s_n & \cdots & s_{n+k} \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{array} \right| \bigg/ \left| \begin{array}{ccc} 1 & \cdots & 1 \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{array} \right|,$$

$$g_{k,j}^{(n)} = \left| \begin{array}{ccc} g_j(n) & \cdots & g_j(n+k) \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{array} \right| \bigg/ \left| \begin{array}{ccc} 1 & \cdots & 1 \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{array} \right|, \quad j > k,$$

respectively.

If we set $c_k^{(n)} = g_{k-1,k}^{(n)} / (g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)})$, then (3) and (4) become

$$E_k^{(n)} = E_{k-1}^{(n)} - c_k^{(n)}(E_{k-1}^{(n+1)} - E_{k-1}^{(n)}), \quad k > 0, \tag{5}$$

$$g_{k,j}^{(n)} = g_{k-1,j}^{(n)} - c_k^{(n)}(g_{k-1,j}^{(n+1)} - g_{k-1,j}^{(n)}), \quad k > 0, j > k, \tag{6}$$

respectively.

For given s_0, \dots, s_N , the computation of $E_k^{(n-k)}$, $0 \leq n \leq N$, $0 \leq k \leq n$, requires $\frac{1}{3}N^3 + O(N^2)$ $g_{k,j}^{(n)}$'s. The number of operation counts for the E -algorithm, as mentioned in [1], is $\frac{5}{3}N^3 + O(N^2)$, while that with the implementation using (5) and (6) becomes $N^3 + O(N^2)$. More precisely, the latter is $N^3 + \frac{5}{2}N^2 + \frac{3}{2}N$.

We remark that Ford and Sidi [4] implemented the E -algorithm by rewriting in the forms

$$E_k^{(n)} = \frac{E_{k-1}^{(n+1)} - c_k^{(n)}E_{k-1}^{(n)}}{d_k^{(n)}}, \quad k > 0, \tag{7}$$

$$g_{k,j}^{(n)} = \frac{g_{k-1,j}^{(n+1)} - c_k^{(n)}g_{k-1,j}^{(n)}}{d_k^{(n)}}, \quad k > 0, j > k, \tag{8}$$

where $c_k^{(n)} = g_{k-1,k}^{(n+1)} / g_{k-1,k}^{(n)}$, and $d_k^{(n)} = 1 - c_k^{(n)}$. The implementation using (7) and (8) requires exactly the same number of arithmetic operations as that using (5) and (6). However, one can avoid the loss of significant figures by using (5) and (6).

2.2. The Ford–Sidi algorithm

The Ford–Sidi algorithm is defined as follows. Let $u = (u_n)$ be one of sequences $s = (s_n)$, 1, or $g_j = (g_j(n))$. The quantities $\psi_k^{(n)}(u)$ are defined by

$$\psi_0^{(n)}(u) = \frac{u_n}{g_1(n)}, \tag{9}$$

$$\psi_k^{(n)}(u) = \frac{\psi_{k-1}^{(n+1)}(u) - \psi_{k-1}^{(n)}(u)}{\psi_{k-1}^{(n+1)}(g_{k+1}) - \psi_{k-1}^{(n)}(g_{k+1})}, \quad k > 0. \tag{10}$$

Ford and Sidi [4] proved the following theorem using Sylvester’s determinantal identity.

Theorem 2. For $n = 0, 1, \dots$, and $k = 1, 2, \dots$, $\psi_k^{(n)}(u)$ are represented as

$$\psi_k^{(n)}(u) = \frac{\begin{vmatrix} u_n & \cdots & u_{n+k} \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}{\begin{vmatrix} g_{k+1}(n) & \cdots & g_{k+1}(n+k) \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}.$$

By Theorems 1 and 2, $T_k^{(n)}$ can be evaluated by

$$T_k^{(n)} = \frac{\psi_k^{(n)}(s)}{\psi_k^{(n)}(1)}. \tag{11}$$

Following the implementation by Ford and Sidi [4], the computation of $T_k^{(n-k)}$, $0 \leq n \leq N$, $0 \leq k \leq n$, requires $\frac{1}{3}N^3 + \frac{3}{2}N^2 + \frac{7}{6}N$ subtractions, and $\frac{1}{3}N^3 + \frac{5}{2}N^2 + \frac{25}{6}N + 2$ divisions, a total of $\frac{2}{3}N^3 + 4N^2 + \frac{16}{3}N + 2$ arithmetic operations.

Remark. (1) The Ford–Sidi algorithm requires g_{k+1} for computing $\psi_k^{(n)}$. However, for computing $T_k^{(n)}$ the Ford–Sidi algorithm does not require g_{k+1} . The reason is as follows: Let a_1, \dots, a_{k+1} be any sequence such that

$$\begin{vmatrix} a_1 & \cdots & a_{k+1} \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix} \neq 0.$$

Let

$$\bar{\psi}_k^{(n)}(u) = \frac{\begin{vmatrix} u_1 & \cdots & u_{k+1} \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}{\begin{vmatrix} a_1 & \cdots & a_{k+1} \\ g_1(n) & \cdots & g_1(n+k) \\ \cdots & & \cdots \\ g_k(n) & \cdots & g_k(n+k) \end{vmatrix}}.$$

Then by (11) we have

$$T_k^{(n)} = \frac{\bar{\psi}_k^{(n)}(s)}{\bar{\psi}_k^{(n)}(1)}.$$

Using the above trick, when s_0, \dots, s_N , g_1, \dots, g_N are given, we can determine all the $T_k^{(n)}$, $0 \leq n + k \leq N$, by the Ford–Sidi algorithm.

(2) Moreover, neither the value of g_{k+1} nor sequence a_1, \dots, a_{k+1} is required in computing $T_k^{(n)}$, when we use

$$T_k^{(n)} = \frac{\psi_{k-1}^{(n+1)}(s) - \psi_{k-1}^{(n)}(s)}{\psi_{k-1}^{(n+1)}(1) - \psi_{k-1}^{(n)}(1)},$$

which is derived from (10) and (11). The implementation of this fact is just the efficient Ford–Sidi algorithm described in Section 4 of this paper.

3. Mathematical equivalence of the E -algorithm and the Ford–Sidi algorithm

3.1. The Ford–Sidi algorithm is derived from the E -algorithm

Let $u = (u_n)$ be any sequence. Suppose that the sequence transformations $E_k : u = (u_n) \mapsto E_k(u) = (E_k^{(n)}(u))$ are defined by

$$E_0^{(n)}(u) = u_n, \tag{12}$$

$$E_k^{(n)}(u) = \frac{E_{k-1}^{(n)}(u)E_{k-1}^{(n+1)}(g_k) - E_{k-1}^{(n+1)}(u)E_{k-1}^{(n)}(g_k)}{E_{k-1}^{(n+1)}(g_k) - E_{k-1}^{(n)}(g_k)}, \quad k > 0. \tag{13}$$

Suppose the sequence transformations $\psi_k : u = (u_n) \mapsto \psi_k(u) = (\psi_k^{(n)}(u))$ are defined by

$$\psi_k^{(n)}(u) = \frac{E_k^{(n)}(u)}{E_k^{(n)}(g_{k+1})}, \quad k = 0, 1, \dots \tag{14}$$

Theorem 3. *The quantities $\psi_k^{(n)}(u)$ defined by (14) satisfy (9) and (10).*

Proof. It follows from (12) and (14) that $\psi_0^{(n)}(u) = u_n/g_1(n)$.

Using the mathematical induction on k , it can be easily proved that $E_k^{(n)}(1) = 1$. Thus, we have

$$\psi_k^{(n)}(1) = \frac{1}{E_k^{(n)}(g_{k+1})}, \quad k = 0, 1, \dots \tag{15}$$

By (14), we have

$$\psi_k^{(n)}(g_j) = \frac{E_k^{(n)}(g_j)}{E_k^{(n)}(g_{k+1})}, \quad k = 0, 1, \dots; \quad j = k + 1, k + 2, \dots \tag{16}$$

From (13) and (16), we obtain

$$\begin{aligned} \psi_{k-1}^{(n+1)}(g_{k+1}) - \psi_{k-1}^{(n)}(g_{k+1}) &= \frac{E_{k-1}^{(n+1)}(g_{k+1})}{E_{k-1}^{(n+1)}(g_k)} - \frac{E_{k-1}^{(n)}(g_{k+1})}{E_{k-1}^{(n)}(g_k)} \\ &= \frac{E_{k-1}^{(n)}(g_{k+1})E_{k-1}^{(n+1)}(g_k) - E_{k-1}^{(n+1)}(g_{k+1})E_{k-1}^{(n)}(g_k)}{E_{k-1}^{(n+1)}(g_k) - E_{k-1}^{(n)}(g_k)} \frac{E_{k-1}^{(n)}(g_k) - E_{k-1}^{(n+1)}(g_k)}{E_{k-1}^{(n+1)}(g_k)E_{k-1}^{(n)}(g_k)} \\ &= E_k^{(n)}(g_{k+1}) \left(\frac{1}{E_{k-1}^{(n+1)}(g_k)} - \frac{1}{E_{k-1}^{(n)}(g_k)} \right). \end{aligned} \tag{17}$$

By dividing the both sides of (13) by $E_k^{(n)}(g_{k+1})$, we have

$$\frac{E_k^{(n)}(u)}{E_k^{(n)}(g_{k+1})} = \frac{E_{k-1}^{(n)}(u)/E_{k-1}^{(n)}(g_k) - E_{k-1}^{(n+1)}(u)/E_{k-1}^{(n+1)}(g_k)}{E_k^{(n)}(g_{k+1})(1/E_{k-1}^{(n)}(g_k) - 1/E_{k-1}^{(n+1)}(g_k))},$$

therefore from (14) and (17), we obtain

$$\psi_k^{(n)}(u) = \frac{\psi_{k-1}^{(n+1)}(u) - \psi_{k-1}^{(n)}(u)}{\psi_{k-1}^{(n+1)}(g_{k+1}) - \psi_{k-1}^{(n)}(g_{k+1})}. \quad \square$$

We note that Brezinski and Redivo Zaglia [3] derived the relations (14)–(16) from their definitions of $E_k^{(n)}(u)$ and $\psi_k^{(n)}(u)$.

3.2. The E -algorithm is derived from the Ford–Sidi algorithm

Suppose that the sequence transformations ψ_k satisfy (9) and (10) for any sequence $u = (u_n)$. Let the sequence transformations E_k be defined by

$$E_k^{(n)}(u) = \frac{\psi_k^{(n)}(u)}{\psi_k^{(n)}(1)}. \quad (18)$$

Theorem 4. *The $E_k^{(n)}(u)$ defined by (18) satisfies (12) and (13).*

Proof. Since (10), we have

$$\psi_k^{(n)}(g_{k+1}) = 1.$$

Hence, by the definition (18), we obtain

$$E_k^{(n)}(g_{k+1}) = \frac{1}{\psi_k^{(n)}(1)}. \quad (19)$$

By (18) and (10),

$$\begin{aligned} E_k^{(n)}(u) &= \frac{\psi_k^{(n)}(u)}{\psi_k^{(n)}(1)} = \frac{\psi_{k-1}^{(n+1)}(u) - \psi_{k-1}^{(n)}(u)}{\psi_{k-1}^{(n+1)}(1) - \psi_{k-1}^{(n)}(1)} \\ &= \frac{E_{k-1}^{(n+1)}(u)/E_{k-1}^{(n+1)}(g_k) - E_{k-1}^{(n)}(u)/E_{k-1}^{(n)}(g_k)}{1/E_{k-1}^{(n+1)}(g_k) - 1/E_{k-1}^{(n)}(g_k)} \\ &= \frac{E_{k-1}^{(n+1)}(g_k)E_{k-1}^{(n)}(u) - E_{k-1}^{(n)}(g_k)E_{k-1}^{(n+1)}(u)}{E_{k-1}^{(n+1)}(g_k) - E_{k-1}^{(n)}(g_k)}. \quad \square \end{aligned}$$

By Theorems 3 and 4, we consider that the E -algorithm and the Ford–Sidi algorithm are mathematically equivalent.

4. An efficient implementation for the Ford–Sidi algorithm

Let $\psi_k^{(n)}(u)$ be defined by (9) and (10). By (11) and (10), $T_k^{(n)}$ in Eq. (2) is represented as

$$T_k^{(n)} = \frac{\psi_{k-1}^{(n+1)}(s) - \psi_{k-1}^{(n)}(s)}{\psi_{k-1}^{(n+1)}(1) - \psi_{k-1}^{(n)}(1)}, \quad k > 0. \tag{20}$$

Using (20), the Ford–Sidi algorithm is implemented as follows.

```

{read  $s_0, g_1(0)$ }
 $\psi_0^{(0)}(s) := s_0/g_1(0); \psi_0^{(0)}(1) := 1/g_1(0); T_0^{(0)} := s_0;$ 
{save  $T_0^{(0)}, \psi_0^{(0)}(s), \psi_0^{(0)}(1)$ }
{read  $s_1, g_1(1)$ }
 $\psi_0^{(1)}(s) := s_1/g_1(1); \psi_0^{(1)}(1) := 1/g_1(1); T_0^{(1)} := s_1;$ 
 $TN := \psi_0^{(1)}(s) - \psi_0^{(0)}(s); TD := \psi_0^{(1)}(1) - \psi_0^{(0)}(1); T_1^{(0)} := TN/TD;$ 
{save  $T_0^{(1)}, T_1^{(0)}, \psi_0^{(1)}(s), \psi_0^{(1)}(1), TN, TD, \text{discard } \psi_0^{(0)}(s), \psi_0^{(0)}(1)$ }
for  $n := 2$  to  $N$  do
begin
  {read  $s_n, g_j(n), 1 \leq j \leq n - 1, g_n(m), 0 \leq m \leq n$ }
  for  $j := 2$  to  $n - 1$  do  $\psi_0^{(n)}(g_j) := g_j(n)/g_1(n);$ 
  for  $m := 0$  to  $n$  do  $\psi_0^{(m)}(g_n) := g_n(m)/g_1(m);$ 
  for  $k := 1$  to  $n - 2$  do for  $m := 0$  to  $n - k - 1$  do
     $\psi_k^{(m)}(g_n) := (\psi_{k-1}^{(m+1)}(g_n) - \psi_{k-1}^{(m)}(g_n))/D_k^{(m)};$ 
     $D_{n-1}^{(0)} := \psi_{n-2}^{(1)}(g_n) - \psi_{n-2}^{(0)}(g_n); \psi_{n-1}^{(0)}(s) := TN/D_{n-1}^{(0)}; \psi_{n-1}^{(0)}(1) := TD/D_{n-1}^{(0)};$ 
     $T_0^{(n)} := s_n; \psi_0^{(n)}(s) := s_n/g_1(n); \psi_0^{(n)}(1) := 1/g_1(n);$ 
  for  $k := 1$  to  $n - 1$  do
    begin
       $D_k^{(n-k)} := \psi_{k-1}^{(n-k+1)}(g_{k+1}) - \psi_{k-1}^{(n-k)}(g_{k+1});$ 
       $\psi_k^{(n-k)}(s) := (\psi_{k-1}^{(n-k+1)}(s) - \psi_{k-1}^{(n-k)}(s))/D_k^{(n-k)};$ 
       $\psi_k^{(n-k)}(1) := (\psi_{k-1}^{(n-k+1)}(1) - \psi_{k-1}^{(n-k)}(1))/D_k^{(n-k)};$ 
       $T_k^{(n-k)} := \psi_k^{(n-k)}(s)/\psi_k^{(n-k)}(1);$ 
      for  $j := k + 2$  to  $n$  do
         $\psi_k^{(n-k)}(g_j) := (\psi_{k-1}^{(n-k+1)}(g_j) - \psi_{k-1}^{(n-k)}(g_j))/D_k^{(n-k)};$ 
      end
       $TN := \psi_{n-1}^{(1)}(s) - \psi_{n-1}^{(0)}(s); TD := \psi_{n-1}^{(1)}(1) - \psi_{n-1}^{(0)}(1); T_n^{(0)} := TN/TD;$ 
      {save  $\psi_k^{(n-k)}(s), \psi_k^{(n-k)}(1), 0 \leq k \leq n - 1, \psi_k^{(n-k)}(g_j), 0 \leq k \leq n - 2,$ 
 $k + 2 \leq j \leq n, TN, TD, \text{discarding all others}$ }
      {save all  $T_k^{(n-k)}, 0 \leq k \leq n, D_k^{(l)}, 1 \leq l + k \leq n, 1 \leq k \leq n - 1$ }
    end;

```

(The **for** statements of the form “**for** $k := k_1$ **to** k_2 **do**” are not executed if $k_1 > k_2$.)

This algorithm will be called the efficient implementation for the Ford–Sidi algorithm. It is clear that this algorithm is mathematically equivalent to the *E*-algorithm and the Ford–Sidi algorithm.

Table 1
The numbers of arithmetic operation counts of three algorithms

Algorithm	Operation counts	$N = 10$	$N = 20$
The E -algorithm using (5) and (6)	$N^3 + \frac{5}{2}N^2 + \frac{3}{2}N$	1265	9030
The Ford–Sidi algorithm	$\frac{2}{3}N^3 + 4N^2 + \frac{16}{3}N + 2$	1122	7042
The present method	$\frac{2}{3}N^3 + 3N^2 + \frac{10}{3}N$	1000	6600

The computation of $T_k^{(n-k)}$, $0 \leq n \leq N$, $0 \leq k \leq n$, by the efficient implementation for the Ford–Sidi algorithm, requires $\frac{1}{3}N^3 + N^2 + \frac{2}{3}N$ subtractions, and $\frac{1}{3}N^3 + 2N^2 + \frac{8}{3}N$ divisions, a total of $\frac{2}{3}N^3 + 3N^2 + \frac{10}{3}N$ arithmetic operations. Although operation counts of the present method and the Ford–Sidi algorithm are asymptotically equal, the present method is slightly more economical than the Ford–Sidi algorithm.

The number of arithmetic operation counts for the computation of $T_k^{(n-k)}$, $0 \leq n \leq N$, $0 \leq k \leq n$, by the E -algorithm using (5) and (6), the Ford–Sidi algorithm, and the present method are listed in Table 1.

Suppose that we accelerate the convergence of a usual sequence by a suitable method such as the Levin u transform in double precision, and that $T_N^{(0)}$ is an optimal extrapolated value. Then it is usually $10 \leq N \leq 20$. (See, for example, [2,7].) Therefore, by Table 1, the present method is, in practice, 6–11% more economical than the Ford–Sidi algorithm.

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Diophantine approximations using Padé approximations

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Abstract

We show how Padé approximations are used to get Diophantine approximations of real or complex numbers, and so to prove the irrationality. We present two kinds of examples. First, we study two types of series for which Padé approximations provide exactly Diophantine approximations. Then, we show how Padé approximants to the asymptotic expansion of the remainder term of a value of a series also leads to Diophantine approximation. © 2000 Elsevier Science B.V. All rights reserved.

1. Preliminary

Definition 1 (*Diophantine approximation*). Let x a real or complex number and $(p_n/q_n)_n$ a sequence of \mathbb{Q} or $\mathbb{Q}(i)$.

If $\lim_{n \rightarrow \infty} |q_n x - p_n| = 0$ and $p_n/q_n \neq x, \forall n \in \mathbb{N}$, then the sequence $(p_n/q_n)_n$ is called a Diophantine approximation of x .

It is well known that Diophantine approximation of x proves the irrationality of x .

So, to construct Diophantine approximation of a number, a mean is to find rational approximation, for example with Padé approximation.

We first recall the theory of formal orthogonal polynomials and its connection with Padé approximation and ε -algorithm.

1.1. Padé approximants

Let h be a function whose Taylor expansion about $t=0$ is $\sum_{i=0}^{\infty} c_i t^i$. The Padé approximant $[m/n]_h$ to h is a rational fraction $N_m(t)/D_n(t)$ whose Taylor series at $t=0$ coincides with that of h up to

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the maximal order, which is in general the sum of the degrees of numerator and denominator of the fraction, i.e,

$$\deg(N_m) \leq m, \quad \deg(D_n) \leq n, \quad D_n(t)h(t) - N_m(t) = O(t^{m+n+1}), \quad t \rightarrow 0.$$

Note that the numerator N_m and the denominator D_n both depend on the index m and n .

The theory of Padé approximation is linked with the theory of orthogonal polynomials (see [10]): Let us define the linear functional c acting on the space \mathcal{P} of polynomials as follows:

$$c : \mathcal{P} \rightarrow \mathbb{R} \quad (\text{or } \mathbb{C}),$$

$$x^i \rightarrow \langle c, x^i \rangle = c_i, \quad i = 0, 1, 2, \dots \text{ and if } p \in \mathbb{Z},$$

$$c^{(p)} : \mathcal{P} \rightarrow \mathbb{R} \quad (\text{or } \mathbb{C}),$$

$$x^i \rightarrow \langle c^{(p)}, x^i \rangle := \langle c, x^{i+p} \rangle = c_{i+p}, \quad i = 0, 1, 2, \dots \quad (c_i = 0, i < 0),$$

then the denominators of the Padé approximants $[m/n]$ satisfy the following orthogonality property:

$$\langle c^{(m-n+1)}, x^i \tilde{D}_n(x) \rangle = 0, \quad i = 0, 1, 2, \dots, n-1,$$

where $\tilde{D}_n(x) = x^n D_n(x^{-1})$ is the reverse polynomial. Since the polynomials D_n involved in the expression of Padé approximants depend on the integers m and n , and since \tilde{D}_n is orthogonal with respect to the shifted linear functional $c^{(m-n+1)}$, we denote

$$P_n^{(m-n+1)}(x) = \tilde{D}_n(x),$$

$$\tilde{Q}_n^{(m-n+1)}(x) = N_m(x).$$

If we set

$$R_{n-1}^{(m-n+1)}(t) := \left\langle c^{(m-n+1)}, \frac{P_n^{(m-n+1)}(x) - P_n^{(m-n+1)}(t)}{x-t} \right\rangle, \quad R_{n-1}^{(m-n+1)} \in \mathcal{P}_{n-1},$$

where $c^{(m-n+1)}$ acts on the letter x , then

$$N_m(t) = \left(\sum_{i=0}^{m-n} c_i t^i \right) \tilde{P}_n^{(m-n+1)}(t) + t^{m-n+1} \tilde{R}_{n-1}^{(m-n+1)}(t),$$

where $\tilde{R}_{n-1}^{(m-n+1)}(t) = t^{n-1} R_{n-1}^{(m-n+1)}(t^{-1})$, $\tilde{P}_n^{(m-n+1)}(t) = t^n P_n^{(m-n+1)}(t^{-1})$ and $\sum_{i=0}^{n-m} c_i t^i = 0$, $n < m$.

The sequence of polynomials $(P_k^{(n)})_k$, of degree k , exists if and only if $\forall n \in \mathbb{Z}$, the Hankel determinant

$$H_k^{(n)} := \begin{vmatrix} c_n & \cdots & c_{n+k-1} \\ \cdots & \cdots & \cdots \\ c_{n+k-1} & \cdots & c_{n+2k-2} \end{vmatrix} \neq 0,$$

where $c_n = 0$ if $n < 0$.

In that case, we shall say that the linear functional c is completely definite. For the noncompletely definite case, the interested reader is referred to Draux [15].

For extensive applications of Padé approximants to Physics, see Baker’s monograph [5].

If c admits an integral representation by a nondecreasing function α , with bounded variation

$$c_i = \int_{\mathbb{R}} x^i d\alpha(x),$$

then the theory of Gaussian quadrature shows that the polynomials P_n orthogonal with respect to c , have all their roots in the support of the function α and

$$\begin{aligned} h(t) - [m/n]_h(t) &= \frac{t^{m-n+1}}{(\tilde{P}_n^{(m-n+1)}(t))^2} c^{(m-n+1)} \left(\frac{(\tilde{P}_n^{(m-n+1)}(x))^2}{1-xt} \right) \\ &= \frac{t^{m-n+1}}{(\tilde{P}_n^{(m-n+1)}(t))^2} \int_{\mathbb{R}} x^{m-n+1} \frac{(\tilde{P}_n^{(m-n+1)}(x))^2}{1-xt} d\alpha(x). \end{aligned} \tag{1}$$

Note that if $c_0 = 0$ then $[n/n]_h(t) = t[n-1/n]_{h/t}(t)$ and if $c_0 = 0$ and $c_1 = 0$, then $[n/n]_h(t) = t^2[n-2/n]_{h/t^2}(t)$.

Consequence: If α is a nondecreasing function on \mathbb{R} , then

$$h(t) \neq [m/n]_f(t) \quad \forall t \in \mathbb{C} - \text{supp}(\alpha).$$

1.2. Computation of Padé approximants with ε -algorithm

The values of Padé approximants at some point of parameter t , can be recursively computed with the ε -algorithm of Wynn. The rules are the following:

$$\begin{aligned} \varepsilon_{-1}^{(n)} &= 0, \quad \varepsilon_0^{(n)} = S_n, \quad n = 0, 1, \dots, \\ \varepsilon_{k+1}^{(n)} &= \varepsilon_{k-1}^{(n+1)} + \frac{1}{\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}}, \quad k, n = 0, 1, \dots \quad (\text{rhombus rule}), \end{aligned}$$

where $S_n = \sum_{k=0}^n c_k t^k$.

ε -values are placed in a double-entry array as following:

$$\begin{array}{ccccccc} \varepsilon_{-1}^{(0)} & = & 0 & & & & \\ & & \varepsilon_0^{(0)} & = & S_0 & & \\ \varepsilon_{-1}^{(1)} & = & 0 & & \varepsilon_1^{(0)} & & \\ & & \varepsilon_0^{(1)} & = & S_1 & & \varepsilon_2^{(0)} \\ \varepsilon_{-1}^{(2)} & = & 0 & & \varepsilon_1^{(1)} & & \varepsilon_3^{(0)} \\ & & \varepsilon_0^{(2)} & = & S_2 & & \varepsilon_2^{(1)} & \ddots \\ \varepsilon_{-1}^{(3)} & = & 0 & & \varepsilon_1^{(2)} & & \vdots & \ddots \\ & & \vdots & & \varepsilon_0^{(3)} & = & S_3 & & \vdots & \ddots \end{array}$$

The connection between Padé approximant and ε -algorithm has been established by Shanks [26] and Wynn [35]:

Theorem 2. *If we apply ε -algorithm to the partial sums of the series $h(t) = \sum_{i=0}^{\infty} c_i t^i$, then*

$$\varepsilon_{2k}^{(n)} = [n + k/k]_h(t).$$

Many convergence results for ε -algorithm has been proved for series which are meromorphic functions in some complex domain, or which have an integral representation (Markov–Stieltjes function) (see [29,6,11] for a survey).

2. Diophantine approximation of sum of series with Padé approximation

Sometimes, Padé approximation is sufficient to prove irrationality of values of a series, as it can be seen in the following two results.

2.1. Irrationality of $\ln(1 - r)$

We explain in the following theorem, how the old proof of irrationality of some logarithm number can be re-written in terms of ε -algorithm.

Theorem 3. *Let $r = a/b$, $a \in \mathbb{Z}$, $b \in \mathbb{N}$, $b \neq 0$, with $\text{b.e.}(1 - \sqrt{1 - r})^2 < 1 (\ln e = 1)$ Then ε -algorithm applied to the partial sums of $f(r) := -\ln(1 - r)/r = \sum_{i=0}^{\infty} r^i / (i + 1)$ satisfies that $\forall n \in \mathbb{N}$, $(\varepsilon_{2k}^{(n)})_k$ is a Diophantine approximation of $f(r)$.*

Proof. From the connection between Padé approximation, orthogonal polynomials and ε -algorithm, the following expression holds:

$$\varepsilon_{2k}^{(n)} = \sum_{i=0}^n \frac{r^i}{i + 1} + r^{n+1} \frac{\tilde{R}_{k-1}^{(n+1)}(r)}{\tilde{P}_k^{(n+1)}(r)} = \frac{N_{n+k}(r)}{\tilde{P}_k^{(n+1)}(r)},$$

where

$$\tilde{P}_k^{(n+1)}(t) = t^k P_k^{(n+1)}(t^{-1}) = \sum_{i=0}^k \binom{k}{k-i} \binom{k+n+1}{i} (1-t)^i$$

is the reversed shifted Jacobi polynomial on $[0,1]$, with parameters $\alpha = 0$, $\beta = n + 1$, and $\tilde{R}_{k-1}^{(n+1)}(t) = t^{k-1} R_{k-1}^{(n+1)}(t^{-1})$ with $R_{k-1}^{(n+1)}(t) = \langle c^{(n+1)}, \frac{P_k^{(n+1)}(x) - P_k^{(n+1)}(t)}{x-t} \rangle (\langle c^{(n+1)}, x^i \rangle := 1/(n + i + 2))$ (c acts on the variable x).

Since $\tilde{P}_k^{(n+1)}(t)$ has only integer coefficients, $b^k \tilde{P}_k^{(n+1)}(a/b) \in \mathbb{Z}$.

The expression of $R_{k-1}^{(n+1)}(t)$ shows that $d_{n+k+1} b^k \tilde{R}_{k-1}^{(n+1)}(a/b) \in \mathbb{Z}$, where $d_{n+k+1} := \text{LCM}(1, 2, \dots, n + k + 1)$ (LCM means lowest common multiple).

We prove now that the sequence $(\varepsilon_{2k}^{(n)})_k$ is a Diophantine approximation of $\ln(1 - a/b)$.

The proof needs asymptotics for d_{n+k+1} , for $\tilde{P}_k^{(n+1)}(a/b)$ and for $(\varepsilon_{2k}^{(n)} - f(r))$ when k tends to infinity. $d_n = e^{n(1+o(1))}$ follows from analytic number theory [1].

$\lim_k(\tilde{P}_k^{(n+1)}(x))^{1/k} = x(y + \sqrt{y^2 - 1})$, $x > 1$, $y = 2/x - 1$, comes from asymptotic properties of Jacobi polynomials (see [30]), and $\lim_{k \rightarrow +\infty}(\varepsilon_{2k}^{(n)} - f(r))^{1/k} = (2/r - 1 - \sqrt{(2/r - 1)^2 - 1})^2$ (error of Padé approximants to Markov–Stieltjes function).

So

$$\begin{aligned} & \lim_{k \rightarrow +\infty} \sup \left| d_{n+k+1} b^k \tilde{P}_k^{(n+1)}(a/b) f(r) - d_{n+k+1} b^k N_{n+k}(a/b) \right|^{1/k} \\ & \leq \lim_{k \rightarrow +\infty} \sup (d_{n+k+1})^{1/k} \limsup_k \left| b^k \tilde{P}_k^{(n+1)}(a/b) \right|^{1/k} \lim_{k \rightarrow +\infty} \sup \left| \varepsilon_{2k}^{(n)} + 1/r \ln(1 - r) \right|^{1/k} \\ & \leq \text{e.b.r.} (2/r - 1 + \sqrt{(2/r - 1)^2 - 1})(2/r - 1 - \sqrt{(2/r - 1)^2 - 1})^2 \\ & = \text{e.b.} (2/r - 1 - \sqrt{(2/r - 1)^2 - 1}) = \text{e.b.} (1 - \sqrt{1 - r})^2 < 1 \end{aligned}$$

by hypothesis, which proves that

$$\forall n \in \mathbb{N}, \quad \lim_{k \rightarrow +\infty} (d_{n+k+1} b^k \tilde{P}_k^{(n+1)}(a/b) f(r) - d_{n+k+1} b^k N_{n+k}(a/b)) = 0.$$

Moreover,

$$\varepsilon_{2k}^{(n)} + 1/r \ln(1 - r) = - \frac{r^{2k+n+1}}{(\tilde{P}_k^{(n+1)}(r))^2} \int_0^1 \frac{(P_k^{(n+1)}(x))^2}{1 - xr} (1 - x)^{n+1} dx \neq 0.$$

So the sequence $(\varepsilon_{2k}^{(n)})_k$ is a Diophantine approximation of $\ln(1 - a/b)$, if $\text{b.e.}(1 - \sqrt{1 - a/b})^2 < 1$. □

2.2. Irrationality of $\sum t^n/w_n$

The same method as previously seen provides Diophantine approximations of $f(t) := \sum_{n=0}^{\infty} t^n/w_n$ when the sequence $(w_k)_k$ satisfies a second-order recurrence relation

$$w_{n+1} = sw_n - pw_{n-1}, \quad n \in \mathbb{N}, \tag{2}$$

where w_0 and w_{-1} are given in \mathbb{C} and s and p are some complex numbers.

We suppose that $w_n \neq 0, \forall n \in \mathbb{N}$ and that the two roots of the characteristic equation $z^2 - sz + p = 0$, α and β satisfy $|\alpha| > |\beta|$.

So w_n admits an expression in term of geometric sequences: $w_n = A\alpha^n + B\beta^n, n \in \mathbb{N}$.

The roots of the characteristic equation are assumed to be of distinct modulus ($|\alpha| > |\beta|$), so there exists an integer r such that $|\alpha/\beta|^r > |B/A|$.

Lemma 4 (see [25]). *If α, β, A, B are some complex numbers, and $|\alpha| > |\beta|$, then the function*

$$f(t) := \sum_{k=0}^{\infty} \frac{t^k}{A\alpha^k + B\beta^k}$$

admits another expansion

$$f(t) = \sum_{k=0}^{r-1} \frac{t^k}{A\alpha^k + B\beta^k} - \frac{t^r}{A\alpha^r} \sum_{k=0}^{\infty} \frac{[(-B/A)(\beta/\alpha)^{r-1}]^k}{t/\alpha - (\alpha/\beta)^k},$$

where $r \in \mathbb{N}$ is chosen such that $|\alpha|^r|A| > |\beta|^r|B|$.

With the notations of Section 1.1, the Padé approximant $[n + k - 1/k]_f$ is

$$[n + k - 1/k]_f(t) = \frac{\tilde{Q}_k^{(n)}(t)}{\tilde{P}_k^{(n)}(t)},$$

where $\tilde{P}_k^{(n)}(t) = t^k P_k^{(n)}(t^{-1})$.

In a previous papers by the author [24,25], it has been proved that for all $n \in \mathbb{Z}$, the sequence of Padé approximants $([n + k - 1/k])_k$ to f converges on any compact set included in the domain of meromorphy of the function f , with the following error term:

$$\forall t \in \mathbb{C} \setminus \{\alpha(\alpha/\beta)^j, j \in \mathbb{N}\}, \forall n \in \mathbb{N}, \limsup_k |f(t) - [n + k - 1/k]_f(t)|^{1/k^2} \leq \frac{\beta}{\alpha}, \tag{3}$$

where α and β are the two solutions of $z^2 - sz + p = 0$, $|\alpha| > |\beta|$.

Theorem 5. *If $\tilde{Q}_k^{(n)}(t)/\tilde{P}_k^{(n)}(t)$ denotes the Padé approximant $[n + k - 1/k]_f$, then*

$$(a) \quad \tilde{P}_k^{(n)}(t) = \sum_{i=0}^k \binom{k}{i}_q q^{i(i-1)/2} (-t/\alpha)^i \prod_{j=1}^i \frac{A + Bq^{n+k-j}}{A + Bq^{n+2k-j}},$$

where

$$q := \beta/\alpha, \quad \binom{k}{i}_q := \frac{(1 - q^k) \dots (1 - q^{k-i+1})}{(1 - q)(1 - q^2) \dots (1 - q^i)}, \quad 1 \leq i \leq k \text{ (Gaussian binomial coefficient)},$$

$$\binom{k}{0}_q = 1.$$

$$(b) \quad |\tilde{P}_k^{(n)}(t) - \prod_{j=0}^{k-1} (1 - tq^j/\alpha)| \leq R|q|^k, \quad k \geq K_0$$

for some constant R independent of k and K_0 is an integer depending on A, B, q, n .

Moreover, if $s, p, w_{-1}, w_0 \in \mathbb{Z}(i)$, for all common multiple d_m of $\{w_0, w_1, \dots, w_m\}$

$$(c) \quad w_{n+k} \cdots w_{n+2k-1} \tilde{P}_k^{(n)} \in \mathbb{Z}(i)[t], \quad \forall n \in \mathbb{Z}/n + k - 1 \geq 0$$

and

$$(d) \quad d_{n+k-1} w_{n+k} \cdots w_{n+2k-1} \tilde{Q}_k^{(n)} \in \mathbb{Z}(i)[t], \quad \forall n \in \mathbb{Z} / n+k-1 \geq 0.$$

Proof. (a) is proved in [16] and (b) is proved in [25]. (c) and (d) comes from expression (a). \square

The expression of w_n is

$$w_n = A\alpha^n + B\beta^n.$$

If A or B is equal to 0 then $f(t)$ is a rational function, so without loss of generality, we can assume that $AB \neq 0$.

The degrees of $\tilde{Q}_k^{(n)}$ and $\tilde{P}_k^{(n)}$ are, respectively, $k+n-1$ and k , so if we take $t \in \mathbb{Q}(i)$ with $vt \in \mathbb{Z}(i)$, the above theorem implies that the following sequence:

$$e_{k,n} := f(t) \times v^{k'} d_{n+k-1} w_{n+k} \cdots w_{n+2k-1} \tilde{P}_k^{(n)}(t) - v^{k'} d_{n+k-1} w_{n+k} \cdots w_{n+2k-1} \tilde{Q}_k^{(n)}(t),$$

where $k' = \max\{n+k-1, k\}$ is a Diophantine approximation to $f(t)$, if

- (i) $\forall n \in \mathbb{Z}, \lim_{k \rightarrow \infty} e_{k,n} = 0,$
- (ii) $[n+k-1/k]_f(t) \neq [n+k/k+1]_f(t).$

For sake of simplicity, we only display the proof for the particular case $n = 0$.

We set

$$e_k := e_{k,0}, \quad \tilde{Q}_k := \tilde{Q}_k^{(0)} \quad \text{and} \quad \tilde{P}_k := \tilde{P}_k^{(0)}.$$

From the asymptotics given in (3), we get

$$\limsup_k |e_k|^{1/k^2} \leq \limsup_k \left| f(t) - \frac{\tilde{Q}_k(t)}{\tilde{P}_k(t)} \right|^{1/k^2} \limsup_k \left| v^k d_{k-1} w_k \cdots w_{2k-1} \tilde{P}_k(t) \right|^{1/k^2} \tag{4}$$

$$\leq |p| \limsup_k |\rho_{k-1}|^{1/k^2}, \tag{5}$$

where $\rho_k := d_k / \prod_{i=0}^k w_i$.

We will get $\lim_{k \rightarrow \infty} e_k = 0$ if the following condition is satisfied:

$$\limsup_{k \rightarrow \infty} |\rho_{k-1}|^{1/k^2} < 1/|p|.$$

Moreover, from the Christoffel–Darboux identity between orthogonal polynomials, condition (ii) is satisfied since the difference

$$\tilde{Q}_{k+1}(t)\tilde{P}_k(t) - \tilde{P}_{k+1}(t)\tilde{Q}_k(t) = t^{2k} \frac{(-1)^k}{A+B} \prod_{i=1}^k AB p^{2i-2} (\alpha^i - \beta^i)^2 \frac{w_{i-1}^2}{w_{2i-1}^2 w_{2i} w_{2i-2}^2}$$

is different from 0.

The following theorem is now proved.

Theorem 6. Let f be the meromorphic function defined by the following series:

$$f(t) = \sum_{n=0}^{\infty} \frac{t^n}{w_n},$$

where $(w_n)_n$ is a sequence of $\mathbb{Z}(i)$ satisfying a three-term recurrence relation

$$w_{n+1} = s w_n - p w_{n-1}, \quad s, p \in \mathbb{Z}(i)$$

with the initial conditions: $w_{-1}, w_0 \in \mathbb{Z}(i)$. If for each integer m , there exists a common multiple d_m for the numbers $\{w_0, w_1, \dots, w_m\}$ such that ρ_m defined by

$$\rho_m := \frac{d_m}{\prod_{i=0}^m w_i}$$

satisfies the condition

$$\limsup_m |\rho_m|^{1/m^2} < 1/|p|, \tag{6}$$

then for $t \in \mathbb{Q}(i)$, $t \neq \alpha(\alpha/\beta)^j$, $j = 0, 1, 2, \dots$ we have

$$f(t) \notin \mathbb{Q}(i).$$

See [25] for application to Fibonacci and Lucas series. (If F_n and L_n are, respectively, Fibonacci and Lucas sequences, then $f(t) = \sum t^n/F_n$ and $g(t) = \sum t^n/L_n$ are not rational for all t rational, not a pole of the functions f or g , which is a generalization of [2].)

3. Diophantine approximation with Padé approximation to the asymptotic expansion of the remainder of the series

For sums of series f , Padé approximation to the function f does not always provide Diophantine approximation. Although the approximation error $|x - p_n/q_n|$ is very sharp, the value of the denominator q_n of the approximation may be too large such that $|q_n x - p_n|$ does not tend to zero when n tends to infinity.

Another way is the following.

Consider the series $f(t) = \sum_{i=0}^{\infty} c_i t^i = \sum_{i=0}^n c_i t^i + R_n(t)$. If, for some complex number t_0 , we know the asymptotic expansion of $R_n(t_0)$ on the set $\{1/n^i, i = 1, 2, \dots\}$, then it is possible to construct an approximation of $f(t_0)$, by adding to the partial sums $S_n(t_0) := \sum_{i=0}^n c_i t_0^i$, some Padé approximation to the remainder $R_n(t_0)$ for the variable n .

But it is not sure that we will get a Diophantine approximation for two reasons.

- (1) the Padé approximation to $R_n(t_0)$ may not converge to $R_n(t_0)$,
- (2) the denominator of the approximant computed at t_0 , can converge to infinity more rapidly than the approximation error does converge to zero.

So, this method works only for few cases.

3.1. Irrationality of $\zeta(2), \zeta(3)$, $\ln(1 + \lambda)$ and $\sum_n 1/(q^n + r)$

3.1.1. Zeta function

The Zeta function of Riemann is defined as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \tag{7}$$

where the Dirichlet series on the right-hand side of (7) is convergent for $\text{Re}(s) > 1$ and uniformly convergent in any finite region where $\text{Re}(s) \geq 1 + \delta$, with $\delta > 0$. It defines an analytic function for $\text{Re}(s) > 1$.

Riemann’s formula

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{x^{s-1}}{e^x - 1} dx, \quad \text{Re}(s) > 1,$$

where

$$\Gamma(s) = \int_0^\infty y^{s-1} e^{-y} dy \text{ is the gamma function} \tag{8}$$

and

$$\zeta(s) = \frac{e^{-i\pi s} \Gamma(1-s)}{2i\pi} \int_{\mathcal{C}} \frac{z^{s-1}}{e^z - 1} dz \tag{9}$$

where \mathcal{C} is some path in \mathbb{C} , provides the analytic continuation of $\zeta(s)$ over the whole s -plane.

If we write formula (7) as

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \sum_{k=1}^\infty \frac{1}{(n+k)^s}$$

and set $\Psi_s(x) := \Gamma(s) \sum_{k=1}^\infty (x/(1+kx))^s$ then

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{\Gamma(s)} \Psi_s(1/n). \tag{10}$$

The function $\sum_{k=1}^\infty (x/(1+kx))^s$ is known as the generalized zeta-function $\zeta(s, 1 + 1/x)$ [32, Chapter XIII] and so we get another expression of $\Psi_s(x)$:

$$\Psi_s(x) = \int_0^\infty u^{s-1} \frac{e^{-u/x}}{e^u - 1} du, \quad x > 0,$$

whose asymptotic expansion is

$$\Psi_s(x) = \sum_{k=0}^\infty \frac{B_k}{k!} \Gamma(k+s-1) x^{k+s-1},$$

where B_k are the Bernoulli numbers.

Outline of the method: In (10), we replace the unknown value $\Psi_s(1/n)$ by some Padé-approximant to $\Psi_s(x)$, at the point $x = 1/n$. We get the following approximation:

$$\zeta(s) \approx \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{\Gamma(s)} [p/q]_{\Psi_s}(x = 1/n). \tag{11}$$

We only consider the particular case $p = q$.

Case $\zeta(2)$: If $s = 2$ then (10) becomes

$$\zeta(2) = \sum_{k=1}^n \frac{1}{k^2} + \Psi_2(1/n),$$

and its approximation (11):

$$\zeta(2) \approx \sum_{k=1}^n \frac{1}{k^2} + [p/p]_{\Psi_2}(x = 1/n), \tag{12}$$

where

$$\Psi_2(x) = \sum_{k=0}^{\infty} B_k x^{k+1} = B_0 x + B_1 x^2 + B_2 x^3 + \dots \quad (\text{asymptotic expansion}). \tag{13}$$

The asymptotic expansion (13) is Borel-summable and its sum is

$$\Psi_2(x) = \int_0^{\infty} u \frac{e^{-u/x}}{e^u - 1} du.$$

Computation of $[p/p]_{\Psi_2(x)/x}$: We apply Section 1.1, where function $f(x) = \Psi_2(x)/x$. The Padé approximants $[p/p]_f$ are linked with the orthogonal polynomial with respect to the sequence $B_0, B_1, B_2 \dots$

As in Section 1, we define the linear functional B acting on the space of polynomials by

$$B : \mathcal{P} \rightarrow \mathbb{R}$$

$$x^i \rightarrow \langle B, x^i \rangle = B_i, \quad i = 0, 1, 2, \dots$$

The orthogonal polynomials Ω_p satisfy

$$\langle B, x^i \Omega_p(x) \rangle = 0, \quad i = 0, 1, \dots, p - 1. \tag{14}$$

These polynomials have been studied by Touchard ([31,9,28,29]) and generalized by Carlitz ([12,13]).

The following expressions

$$\begin{aligned} \Omega_p(x) &= \sum_{2r \leq p} \binom{2x + p - 2r}{p - 2r} \binom{x}{r}^2 \\ &= (-1)^p \sum_{k=0}^p (-1)^k \binom{p}{k} \binom{p+k}{k} \binom{x+k}{k} = \sum_{k=0}^p \binom{p}{k} \binom{p+k}{k} \binom{x}{k} \end{aligned} \tag{15}$$

hold (see [34,12]).

Note that the Ω_p 's are orthogonal polynomials and thus satisfy a three-term recurrence relation.

The associated polynomials A_p of degree $p - 1$ are defined as

$$A_p(t) = \left\langle B, \frac{\Omega_p(x) - \Omega_p(t)}{x - t} \right\rangle,$$

where B acts on x .

From expression (15) for Ω_p , we get the following formula for A_p :

$$A_p(t) = \sum_{k=0}^p \binom{p}{k} \binom{p+k}{k} \left\langle B, \frac{\binom{x}{k} - \binom{t}{k}}{x - t} \right\rangle.$$

The recurrence relation between the Bernoulli numbers B_i implies that

$$\left\langle B, \binom{x}{k} \right\rangle = \frac{(-1)^k}{k+1}.$$

Using the expression of the polynomial $((\binom{x}{k} - \binom{t}{k})/(x - t))$ on the Newton basis on $0, 1, \dots, k - 1$,

$$\frac{\binom{x}{k} - \binom{t}{k}}{x - t} = \binom{t}{k} \sum_{i=1}^k \frac{\binom{x}{i-1}}{i \binom{t}{i}},$$

we can write a compact formula for A_p :

$$A_p(t) = \sum_{k=1}^p \binom{p}{k} \binom{p+k}{k} \binom{t}{k} \sum_{i=1}^k \frac{(-1)^{i-1}}{i^2 \binom{t}{i}} \in \mathcal{P}_{p-1}.$$

Approximation (12) for $\zeta(2)$ becomes

$$\zeta(2) \approx \sum_{k=1}^n \frac{1}{k^2} + t \frac{\tilde{A}_p(t)}{\tilde{\Omega}_p(t)} \Big|_{t=1/n} = \sum_{k=1}^n \frac{1}{k^2} + \frac{A_p(n)}{\Omega_p(n)}.$$

Using partial decomposition of $1/\binom{n}{i}$ with respect to the variable n , it is easy to prove that

$$\frac{d_n}{i \binom{n}{i}} \in \mathbb{N}, \quad \forall i \in \{1, 2, \dots, n\} \tag{16}$$

with $d_n := \text{LCM}(1, 2, \dots, n)$.

A consequence of the above result is

$$d_n^2 A_p(n) \in \mathbb{N}, \quad \forall p \in \mathbb{N}$$

and

$$d_n^2 \Omega_p(n) \zeta(2) - d_n^2 (S_n \Omega_p(n) + A_p(n)) \tag{17}$$

is a Diophantine approximation of $\zeta(2)$, for all values of integer p , where S_n denotes the partial sums $S_n = \sum_{k=1}^n 1/k^2$. It remains to estimate the error for the Padé approximation:

$$\Psi_2(t) - [p/p]_{\Psi_2}(t) = \Psi_2(t) - [p - 1/p]_{\Psi_2/t}(t).$$

Touchard found the integral representation for the linear functional B :

$$\langle B, x^k \rangle := B_k = -i \frac{\pi}{2} \int_{\alpha-i\infty}^{\alpha+i\infty} x^k \frac{dx}{\sin^2(\pi x)}, \quad -1 < \alpha < 0.$$

Thus, formula (1) becomes

$$t^{-1}\Psi_2(t) - [p - 1/p]_{\Psi_2/t}(t) = -i\frac{\pi}{2} \frac{t^{2p}}{\tilde{\Omega}_p^2(t)} \int_{x-i\infty}^{x+i\infty} \frac{\Omega_p^2(x)}{1 - xt} \frac{dx}{\sin^2(\pi x)},$$

and we obtain the error for the Padé approximant to Ψ_2 :

$$\Psi_2(t) - [p/p]_{\Psi_2}(t) = -i\frac{\pi}{2} \frac{t}{\Omega_p^2(t^{-1})} \int_{x-i\infty}^{x+i\infty} \frac{\Omega_p^2(x)}{1 - xt} \frac{dx}{\sin^2(\pi x)}$$

and the error for formula (17):

$$d_n^2 \Omega_p(n) \zeta(2) - d_n^2 (S_n \Omega_p(n) + A_p(n)) = -d_n^2 i \frac{\pi}{2n} \frac{1}{\Omega_p(n)} \int_{x-i\infty}^{x+i\infty} \frac{\Omega_p^2(x)}{1 - x/n} \frac{dx}{\sin^2(\pi x)}. \tag{18}$$

If $p = n$, we get Apéry’s numbers [4]:

$$b'_n = \Omega_n(n) = \sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{k}$$

and

$$a'_n = S_n \Omega_n(n) + A_n(n) = \left(\sum_{k=1}^n \frac{1}{k^2} \right) b'_n + \sum_{k=1}^n \binom{n}{k}^2 \binom{n+k}{k} \sum_{i=1}^k \frac{(-1)^{i-1}}{i^2} \binom{n}{i}.$$

The error in formula (18) becomes

$$d_n^2 b'_n \zeta(2) - d_n^2 a'_n = -d_n^2 i \frac{\pi}{2n} \frac{1}{b'_n} \int_{x-i\infty}^{x+i\infty} \frac{\Omega_n^2(x)}{1 - x/n} \frac{dx}{\sin^2 \pi x} \tag{19}$$

In order to prove the irrationality of $\zeta(2)$, we have to show that the right-hand side of (19) tends to 0 when n tends to infinity, and is different from 0, for each integer n .

We have

$$\left| \int_{-1/2-i\infty}^{-1/2+i\infty} \frac{\Omega_n^2(x)}{1 - x/n} \frac{dx}{\sin^2 \pi x} \right| \leq \left| \int_{-\infty}^{+\infty} \frac{\Omega_n^2(-\frac{1}{2} + iu)}{1 + 1/2n} \frac{du}{\cosh^2 \pi u} \right| \leq \frac{1}{1 + 1/2n} |\langle B, \Omega_n^2(x) \rangle|$$

since $\cosh^2 \pi u$ is positive for $u \in \mathbb{R}$ and $\Omega_n^2(-\frac{1}{2} + iu)$ real positive for u real (Ω_n has all its roots on the line $-\frac{1}{2} + i\mathbb{R}$, because $\Omega_n(-\frac{1}{2} + iu)$ is orthogonal with respect to the positive weight $1/\cosh^2 \pi u$ on \mathbb{R}). The quantity $\langle B, \Omega_n^2(x) \rangle$ can be computed from the three term recurrence relation between the Ω'_n s [31]:

$$\langle B, \Omega_n^2(x) \rangle = \frac{(-1)^n}{2n + 1}.$$

The Diophantine approximation (19) satisfies

$$|d_n^2 b'_n \zeta(2) - d_n^2 a'_n| \leq d_n^2 \frac{\pi}{(2n + 1)^2} \times \frac{1}{b'_n}.$$

In [14], it is proved that $b'_n \sim A'((1 + \sqrt{5})/2)^{5n} n^{-1}$ when $n \rightarrow \infty$, for some constant A' . From a result concerning $d_n = \text{LCM}(1, 2, \dots, n)$: ($d_n = e^{(n(1+o(1)))}$), we get

$$\lim_{n \rightarrow \infty} |d_n^2 b'_n \zeta(2) - d_n^2 a'_n| = 0, \tag{20}$$

where $d_n^2 b'_n$ and $d_n^2 a'_n$ are integers.

Relation (20) proves that $\zeta(2)$ is not rational.

Case $\zeta(3)$: If $s = 3$ then equality (10) becomes

$$\zeta(3) = \sum_{k=1}^n \frac{1}{k^3} + \frac{1}{2} \Psi_3(1/n), \tag{21}$$

where

$$\Psi_3(x) = \int_0^\infty u^2 \frac{e^{-u/x}}{e^u - 1} du$$

whose asymptotic expansion is

$$\Psi_3(x) = \sum_{k=0}^\infty B_k (k + 1) x^{k+2}.$$

Computation of $[p/p]_{\Psi_3(x)/x^2}$: Let us define the derivative of B by

$$\langle -B', x^k \rangle := \langle B, kx^{k-1} \rangle = kB_{k-1}, \quad k \geq 1,$$

$$\langle -B', 1 \rangle := 0.$$

So, the functional B' admits an integral representation:

$$\langle B', x^k \rangle = i\pi^2 \int_{\alpha-i\infty}^{\alpha+i\infty} x^k \frac{\cos(\pi x)}{\sin^3(\pi x)} dx, \quad -1 < \alpha < 0.$$

Let $(\Pi_n)_n$ be the sequence of orthogonal polynomial with respect to the sequence

$$-B'_0 := 0, \quad -B'_1 = B_0, \quad -B'_2 = 2B_1, \quad -B'_3 = 3B_2, \dots$$

The linear form B' is not definite and so the polynomials Π_n are not of exact degree n .

More precisely, Π_{2n} has degree $2n$ and $\Pi_{2n+1} = \Pi_{2n}$. For the general theory of orthogonal polynomials with respect to a nondefinite functional, the reader is referred to Draux [15]. If we take $\alpha = -\frac{1}{2}$, the weight $\cos \pi x / \sin^3(\pi x) dx$ on the line $-\frac{1}{2} + i\mathbb{R}$ becomes $\sinh \pi t / \cosh^3 \pi t dt$ on \mathbb{R} , which is symmetrical around 0. So, $\Pi_{2n}(it - \frac{1}{2})$ only contains even power of t and we can write

$\Pi_{2n}(it - \frac{1}{2}) = W_n(t^2)$, W_n of exact degree n . Thus W_n satisfies

$$\int_{\mathbb{R}} W_n(t^2) W_m(t^2) \frac{t \sinh \pi t}{\cosh^3 \pi t} dt = 0, \quad n \neq m.$$

The weight $t \sinh \pi t / \cosh^3 \pi t$ equals $(1/4\pi^3) |\Gamma(\frac{1}{2} + it)|^8 |\Gamma(2it)|^2$ and has been studied by Wilson [33,3]:

$$n \geq 0, \quad \Pi_{2n}(y) = \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \binom{y+k}{k} \binom{y}{k}. \tag{22}$$

Let Θ_{2n} the polynomial associated to Π_{2n} :

$$\Theta_{2n}(t) = \left\langle -B', \frac{\Pi_{2n}(x) - \Pi_{2n}(t)}{x - t} \right\rangle, \quad B' \text{ acts on } x.$$

For the computation of Θ_{2n} , we need to expand the polynomial

$$\frac{\binom{x+k}{k} \binom{x}{k} - \binom{t+k}{k} \binom{t}{k}}{x - t}.$$

On the Newton basis with the abscissa $\{0, 1, -1, \dots, n, -n\}$

$$\frac{\binom{x+k}{k} \binom{x}{k} - \binom{t+k}{k} \binom{t}{k}}{x - t} = \sum_{i=1}^{2k} \frac{N_{2k}(t)}{N_i(t)} \frac{N_{i-1}(x)}{[(i+1)/2]},$$

where $N_0(x) := 1$, $N_1(x) = \binom{x}{1}$, $N_2(x) = \binom{x}{1} \binom{x+1}{1}$, \dots , $N_{2i}(x) = \binom{x}{i} \binom{x+i}{i}$, $N_{2i+1}(x) = \binom{x}{i+1} \binom{x+i}{i}$.

By recurrence, the values $\langle -B', N_i(x) \rangle$ can be found in

$$i \in \mathbb{N}, \quad \langle -B', N_{2i}(x) \rangle = 0, \quad \langle -B', N_{2i+1}(x) \rangle = \frac{(-1)^i}{(i+1)^2}.$$

Using the linearity of B' , we get the expression of Θ_{2n} :

$$\Theta_{2n}(t) = \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \sum_{i=1}^k \frac{(-1)^{i+1}}{i^3} \frac{\binom{t+k}{k-i} \binom{t-i}{k-i}}{\binom{k}{i}^2} \in \mathcal{P}_{2n-2}. \tag{23}$$

Eq. (16) implies that

$$d_n^3 \Theta_{2n}(t) \in \mathbb{N}, \quad \forall t \in \mathbb{N}.$$

The link between Π_{2n} , Θ_{2n} and the Apéry's numbers a_n, b_n is given by taking $y = n$ in (22) and $t = n$ in (23):

$$\Pi_{2n}(n) = \sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{k}^2 = b_n,$$

$$\left(\sum_{k=1}^n \frac{1}{k^3} \right) \Pi_{2n}(n) + \frac{1}{2} \Theta_{2n}(n) = a_n.$$

Apéry was the first to prove irrationality of $\zeta(3)$. He only used recurrence relation between the a_n and b_n . We end the proof of irrationality of $\zeta(3)$ with the error term for the Padé approximation.

Let us recall equality (21),

$$\zeta(3) = \sum_{k=1}^n \frac{1}{k^3} + \frac{1}{2} \Psi_3 \left(\frac{1}{n} \right)$$

in which we replace the unknown term $\Psi_3(1/n)$ by its Padé approximant $[2n/2n]_{\Psi_3}(x=1/n)$. It arises the following approximation for $\zeta(3)$:

$$\zeta(3) \approx \sum_{k=1}^n \frac{1}{k^3} + \frac{1}{2} \frac{\Theta_{2n}(n)}{\Pi_{2n}(n)}$$

and the expression

$$e_n = 2d_n^3 \Pi_{2n}(n) \zeta(3) - \left[\left(\sum_{k=1}^n \frac{1}{k^3} \right) 2\Pi_{2n}(n) + \Theta_{2n}(n) \right] d_n^3$$

will be a Diophantine approximation, if we prove that $\lim_n e_n = 0$ (since $\Pi_{2n}(n)$ and $d_n^3 \Theta_{2n}(n)$ are integer).

Let us estimate the error e_n . The method is the same as for $\zeta(2)$:

$$\Psi_3(t) - [2n/2n]_{\Psi_3}(t) = \Psi_3(t) - t^2 [2n - 2/2n]_{\Psi_3/t^2}(t) = \Psi_3(t) - \frac{\Theta_{2n}(t^{-1})}{\Pi_{2n}(t^{-1})}.$$

The integral representation of B' gives

$$\Psi_3(t) - [2n/2n]_{\Psi_3}(t) = -\frac{t\pi^2 i}{\Pi_{2n}^2(t^{-1})} \int_{x-i\infty}^{x+i\infty} \frac{\Pi_{2n}^2(x) \cos \pi x}{1 - xt \sin^3 \pi x} dx.$$

The previous expression implies that the error $\Psi_3(t) - [2n/2n]_{\Psi_3}(t)$ is nonzero, and also that

$$|\Psi_3(t) - [2n/2n]_{\Psi_3}(t)| \leq \frac{\pi^2 t}{\Pi_{2n}^2(t^{-1})} \cdot \frac{1}{1 + t/2} \cdot \int_{\mathbb{R}} W_n^2(u^2) \frac{u \sinh \pi u}{\cosh^3 \pi u} du, \quad t \in \mathbb{R}^+.$$

From the expression of the integral (see [33]) we get

$$|\Psi_3(1/n) - [2n/2n]_{\Psi_3}(1/n)| \leq \frac{4\pi^2}{(2n + 1)^2 \Pi_{2n}^2(n)}.$$

The error term in the Padé approximation satisfies

$$\left| 2\zeta(3) - 2 \sum_{k=1}^n \frac{1}{k^3} - [2n/2n]_{\Psi_3}(1/n) \right| \leq \frac{4\pi^2}{(2n + 1)^2 \Pi_{2n}^2(n)}$$

and the error term e_n satisfies

$$|e_n| = \left| 2d_n^3 \Pi_{2n}(n) \zeta(3) - \left[2 \left(\sum_{k=1}^n \frac{1}{k^3} \right) \Pi_{2n}(n) + \Theta_{2n}(n) \right] d_n^3 \right| \leq \frac{8\pi^2}{(2n + 1)^2} \frac{d_n^3}{\Pi_{2n}(n)}.$$

$\Pi_{2n}(n) = b_n$ implies that $\Pi_{2n}(n) = A(1 + \sqrt{2})^{4n} n^{-3/2}$ [14], and so we get, since $d_n = e^{n(1+o(1))}$,

$$\begin{aligned} |2d_n^3 b_n \zeta(3) - 2d_n^3 a_n| &\rightarrow 0, \\ n &\rightarrow \infty, \end{aligned} \tag{24}$$

where $2d_n^3 b_n$ and $2d_n^3 a_n$ are integers.

The above relation (24) shows that $\zeta(3)$ is irrational.

Of course, using the connection between Padé approximation and ε -algorithm, the Diophantine approximation of $\zeta(3)$ can be constructed by means of the following ε -array: $a_n/b_n = \sum_{k=1}^n 1/k^3 + \varepsilon_{4n}^{(0)}(T_m) = \varepsilon_{4n}^{(0)}(\sum_{k=1}^n 1/k^3 + T_m)$, where T_m is the partial sum of the asymptotic series (nonconvergent) $T_m = \frac{1}{2} \sum_{k=1}^m B_k(k+1)1/n^k$.

We get the following ε -arrays for $n = 1$,

$$\begin{bmatrix} 0 \\ 0 & 0 \\ 1 & 1/2 & 2/5 = \varepsilon_4^{(0)} \\ 0 & 1/3 \\ 1/2 \end{bmatrix}, \quad 1 + \frac{1}{2} * \varepsilon_4^{(0)} = \frac{6}{5} = a_1/b_1 \quad (\text{Apery's numbers}),$$

and for $n = 2$,

$$\begin{bmatrix} 0 \\ 0 & 0 \\ 1/4 & 1/6 & 2/13 \\ 1/8 & 3/20 & 2/13 & 2/13 \\ 5/32 & 5/32 & 21/136 & 37/240 & 45/292 = \varepsilon_8^{(0)} \\ 5/32 & 5/32 & 2/13 & 53/344 \\ 59/384 & 59/384 & 37/240 \\ 59/384 & 59/384 \\ 79/512 \end{bmatrix}$$

(we have only displayed the odd columns), $1 + 1/2^3 + 1/2 * \varepsilon_8^{(0)} = 351/292 = a_2/b_2$. ε -algorithm is a particular extrapolation algorithm as Padé approximation is particular case of Padé-type approximation. Generalization has been achieved by Brezinski and Hävie, the so-called E-algorithm. Diophantine approximation using E-algorithm and Padé-type approximation are under consideration.

3.1.2. Irrationality of $\ln(1 + \lambda)$

In this part, we use the same method as in the preceding section:

$$\text{We set } \ln(1 + \lambda) = \sum_{k=1}^n (-1)^{k+1} \frac{\lambda^k}{k} + \sum_{k=1}^{\infty} \frac{(-1)^{k+n+1}}{k+n} \lambda^{k+n}. \tag{25}$$

From the formula $1/(k + n) = \int_0^\infty e^{-(k+n)v} dv$, we get an integral representation for the remainder term in (25):

$$\sum_{k=1}^{\infty} (-1)^{k+n+1} \frac{\lambda^{k+n}}{k+n} = (-1)^n \int_0^\infty \lambda^{n+1} \frac{e^{-nv}}{e^v + \lambda} dv.$$

If we expand the function

$$\frac{1 + \lambda}{e^v + \lambda} = \sum_{k=0}^{\infty} R_k(-\lambda) \frac{v^k}{k!},$$

where the $R_k(-\lambda)$'s are the Eulerian numbers [12], we get the following asymptotic expansion:

$$\sum_{k=1}^{\infty} (-1)^{k+n+1} \frac{\lambda^{k+n}}{k+n} = \frac{(-1)^n \lambda^{n+1}}{n(1+\lambda)} \left(\sum_{k=0}^{\infty} R_k(-\lambda) x^k \right)_{x=1/n}.$$

Let us set

$$\Phi_1(x) = \sum_{k=0}^{\infty} R_k(-\lambda) x^k.$$

Carlitz has studied the orthogonal polynomials with respect to $R_0(-\lambda), R_1(-\lambda), \dots$.

If we define the linear functional R by

$$\langle R, x^k \rangle := R_k(-\lambda),$$

then the orthogonal polynomials P_n with respect to R , i.e.,

$$\langle R, x^k P_n(x) \rangle = 0, \quad k = 0, 1, \dots, n - 1,$$

satisfy $P_n(x) = \sum_{k=0}^n (1 + \lambda)^k \binom{n}{k} \binom{x}{k}$ [12].

The associated polynomials are

$$Q_n(t) = \sum_{k=0}^n (1 + \lambda)^k \binom{n}{k} \left\langle R, \frac{\binom{x}{k} - \binom{t}{k}}{x - t} \right\rangle. \tag{26}$$

Carlitz proved that $\langle R, \binom{x}{k} \rangle = (-\lambda - 1)^{-k}$ and thus, using (26),

$$Q_n(t) = \sum_{k=0}^n (1 + \lambda)^k \binom{n}{k} \binom{t}{k} \sum_{i=1}^k \frac{1}{i \binom{t}{i}} \left(\frac{-1}{\lambda + 1} \right)^{i-1}.$$

If we set $\lambda = p/q$, p and $q \in \mathbb{Z}$ and $t = n$, then

$$q^n d_n Q_n(n) \in \mathbb{Z}.$$

An integral representation for $R_k(-\lambda)$ is given by Carlitz:

$$R_k(-\lambda) = -\frac{1 + \lambda}{2i\lambda} \int_{\alpha-i\infty}^{\alpha+i\infty} z^k \frac{\lambda^{-z}}{\sin \pi z} dz, \quad -1 < \alpha < 0, \tag{27}$$

and thus

$$\Phi_1(x) = -\frac{1 + \lambda}{2i\lambda} \int_{\alpha-i\infty}^{\alpha+i\infty} \frac{1}{1 - xz} \frac{\lambda^{-z}}{\sin \pi z} dz.$$

The orthogonal polynomial P_n satisfies [12]

$$\int_{\alpha-i\infty}^{\alpha+i\infty} P_n^2(z) \frac{\lambda^{-z}}{\sin \pi z} dz = \frac{+2i}{i + \lambda} (-\lambda)^{n+1},$$

and since $\operatorname{Re}(\lambda^{-z} \sin \pi z) > 0$ for $z \in -\frac{1}{2} + i\mathbb{R}$, we obtain a majoration of the error for the Padé approximation to Φ_1 :

$$x > 0, |\Phi_1(x) - [n - 1/n]_{\Phi_1}(x)| \leq \frac{\lambda^n}{|1 + x/2|}$$

and if $x = 1/n$, we get

$$\left| \Phi_1\left(\frac{1}{n}\right) - [n - 1/n]_{\Phi_1}(1/n) \right| \leq \frac{|\lambda|^n}{1 + 1/2n}.$$

Let us replace in (25) the remainder term by its Padé approximant:

$$\ln(1 + \lambda) \approx \sum_{k=1}^n (-1)^{k+1} \frac{\lambda^k}{k} + \frac{(-1)^n \lambda^{n+1}}{(1 + \lambda)n} [n - 1/n]_{\Phi_1}(1/n),$$

we obtain a Diophantine approximation for $\ln(1 + p/q)$:

$$\left| \ln\left(1 + \frac{p}{q}\right) d_n q^{2n} P_n(n) - d_n q^{2n} T_n(n) \right| \leq \frac{\lambda^{2n} d_n q^{2n}}{(n + 2)P_n(n)}, \tag{28}$$

where $T_n(n) = P_n(n) \sum_{k=1}^n (-1)^{k+1} p^k/kq^k + (-1)^{n+1} Q_n(n)q^n$.

From the expression of $P_n(x)$ we can conclude that

$$P_n(n) = \sum_{k=0}^n (1 + \lambda)^k \binom{n}{k} = \operatorname{Legendre}\left(n, \frac{2}{\lambda} + 1\right) \lambda^n,$$

where $\operatorname{Legendre}(n, x)$ is the n th Legendre polynomial and thus

$$\frac{T_n(n)}{P_n(n)} = [n/n]_{\ln(1+x)}(x = 1).$$

So, the classical proof for irrationality of $\ln(1 + p/q)$ based on Padé approximants to the function $\ln(1 + x)$ is recovered by formula (28).

Proof of irrationality of $\zeta(2)$ with alternated series: Another expression for $\zeta(2)$ is

$$\zeta(2) = 2 \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^2}.$$

Let us write it as a sum

$$\zeta(2) = 2 \sum_{k=1}^n \frac{(-1)^{k-1}}{k^2} + 2 \sum_{k=1}^{\infty} \frac{(-1)^{k+n+1}}{(k + n)^2}.$$

Let Φ_2 be defined by $\Phi_2(x) = \sum_{k=0}^{\infty} R_k(-1)(k + 1)x^k$. So

$$\zeta(2) = 2 \sum_{k=1}^n \frac{(-1)^{k-1}}{k^2} + \frac{(-1)^n}{n^2} \Phi_2(1/n).$$

With the same method, we can prove that the Padé approximant $[2n/2n]_{\Phi_2}(x)$ computed at $x = 1/n$ leads to Apéry’s numbers a'_n and b'_n and so proves the irrationality of $\zeta(2)$ with the

integral representation for the sequence $(kR_{k-1}(-1))_k$:

$$kR_{k-1}(-1) = -\frac{\pi(1 + \lambda)}{2i\lambda} \int_{x-i\infty}^{x+i\infty} z^k \frac{\cos \pi z}{\sin^2 \pi z} dz, \quad k \geq 1.$$

obtained with an integration by parts applied to (27).

3.1.3. Irrationality of $\sum 1/(q^n + r)$

In [7], Borwein proves the irrationality of $L(r) = \sum 1/(q^n - r)$, for q an integer greater than 2, and r a non zero rational (different from q^n , for any $n \geq 1$), by using similar method. It is as follows:

Set

$$L_q(x) := \sum_{n=1}^{\infty} \frac{x}{q^n - x} = \sum_{n=1}^{\infty} \frac{x^n}{q^n - 1}, \quad |q| > 1.$$

Fix N a positive integer and write $L_q(r) = \sum_{n=1}^N r/(q^n - r) + L_q(r/q^N)$.

Then, it remains to replace $L_q(r/q^N)$ by its Padé approximant $[N/N]_{L_q}(r/q^N)$.

The convergence of $[N/N]_{L_q}$ to L_q is a consequence of the following formula:

$$\forall t \in \mathbb{C} \setminus \{q^j, j \in \mathbb{N}\}, \quad \forall n \in \mathbb{N}, \quad \limsup_N |L_q(t) - [N/N]_{L_q}(t)|^{1/3N^2} \leq 1/q.$$

p_n/q_n defined by $p_n/q_n := \sum_{n=1}^N r/(q^n - r) + [N/N]_{L_q}(r/q^N)$ leads to Diophantine approximation of $L_q(r)$ and so proves the irrationality of $L_q(r)$.

For further results concerning the function L_q , see [17–19].

Different authors used Padé or Padé Hermite approximants to get Diophantine approximation, see for example [8,20–23,27].

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The generalized Richardson extrapolation process GREP⁽¹⁾ and computation of derivatives of limits of sequences with applications to the $d^{(1)}$ -transformation

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Abstract

Let $\{S_m\}$ be an infinite sequence whose limit or antilimit S can be approximated very efficiently by applying a suitable extrapolation method E_0 to $\{S_m\}$. Assume that the S_m and hence also S are differentiable functions of some parameter ξ , $(d/d\xi)S$ being the limit or antilimit of $\{(d/d\xi)S_m\}$, and that we need to approximate $(d/d\xi)S$. A direct way of achieving this would be by applying again a suitable extrapolation method E_1 to the sequence $\{(d/d\xi)S_m\}$, and this approach has often been used efficiently in various problems of practical importance. Unfortunately, as has been observed at least in some important cases, when $(d/d\xi)S_m$ and S_m have essentially different asymptotic behaviors as $m \rightarrow \infty$, the approximations to $(d/d\xi)S$ produced by this approach, despite the fact that they are good, do not converge as quickly as those obtained for S , and this is puzzling. In a recent paper (A. Sidi, Extrapolation methods and derivatives of limits of sequences, *Math. Comp.*, 69 (2000) 305–323) we gave a rigorous mathematical explanation of this phenomenon for the cases in which E_0 is the Richardson extrapolation process and E_1 is a generalization of it, and we showed that the phenomenon has nothing to do with numerics. Following that we proposed a very effective procedure to overcome this problem that amounts to first applying the extrapolation method E_0 to $\{S_m\}$ and then differentiating the resulting approximations to S . As a practical means of implementing this procedure we also proposed the direct differentiation of the recursion relations of the extrapolation method E_0 used in approximating S . We additionally provided a thorough convergence and stability analysis in conjunction with the Richardson extrapolation process from which we deduced that the new procedure for $(d/d\xi)S$ has practically the same convergence properties as E_0 for S . Finally, we presented an application to the computation of integrals with algebraic/logarithmic endpoint singularities via the Romberg integration. In this paper we continue this research by treating Sidi's generalized Richardson extrapolation process GREP⁽¹⁾ in detail. We then apply the new procedure to various infinite series of logarithmic type (whether convergent or divergent) in conjunction with the $d^{(1)}$ -transformation of Levin and Sidi. Both the theory and the numerical results of this paper too indicate that this approach is the preferred one for computing derivatives of limits of infinite sequences and series. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction and review of recent developments

Let $\{S_m\}$ be an infinite sequence whose limit or antilimit S can be approximated very efficiently by applying a suitable extrapolation method E_0 to $\{S_m\}$. Assume that the S_m and hence also S are differentiable functions of some parameter ξ , $(d/d\xi)S$ being the limit or antilimit of $\{(d/d\xi)S_m\}$, and that we need to approximate $(d/d\xi)S$. A direct way of achieving this would be by applying again a suitable extrapolation method E_1 to the sequence $\{(d/d\xi)S_m\}$, and this approach has often been used efficiently in various problems of practical importance. When S_m and $(d/d\xi)S_m$ have essentially different asymptotic behaviors as $m \rightarrow \infty$, the approximations to $(d/d\xi)S$ produced by applying E_1 to $\{(d/d\xi)S_m\}$ do not converge to $(d/d\xi)S$ as quickly as the approximations to S obtained by applying E_0 to $\{S_m\}$ even though they may be good. This is a curious and disturbing phenomenon that calls for an explanation and a befitting remedy, and both of these issues were addressed by the author in the recent paper [14] via the Richardson extrapolation. As far as is known to us [14] is the first work that handles this problem.

The procedure to cope with the problem above that was proposed in [14] amounts to *first applying the extrapolation method E_0 to $\{S_m\}$ and then differentiating the resulting approximations to S* . As far as practical implementation of this procedure is concerned, it was proposed in [14] to *actually differentiate the recursion relations satisfied by the method E_0* .

In the present work we continue this new line of research by extending the approach of [14] to GREP⁽¹⁾ that is the simplest case of the generalized Richardson extrapolation process GREP of Sidi [7]. Following this, we consider the application of the $d^{(1)}$ -transformation, the simplest of the d -transformations of Levin and Sidi [6], to computing derivatives of sums of infinite series. Now GREP is a most powerful extrapolation procedure that can be applied to a very large class of sequences and the d -transformations are GREPs that can be applied successfully again to a very large class of infinite series. Indeed, it is known theoretically and has been observed numerically that GREP in general and the d -transformations in particular have scopes larger than most known extrapolation methods.

Before we go on to the main theme of this paper, we will give a short review of the motivation and results of [14]. This will also help establish some of the notation that we will use in the remainder of this work and set the stage for further developments. As we did in [14], here too we will keep the treatment general by recalling that infinite sequences are either directly related to or can be formally associated with a function $A(y)$, where y may be a continuous or discrete variable.

Let a function $A(y)$ be known and hence computable for $y \in (0, b]$ with some $b > 0$, the variable y being continuous or discrete. Assume, furthermore, that $A(y)$ has an asymptotic expansion of the form

$$A(y) \sim A + \sum_{k=1}^{\infty} \alpha_k y^{\sigma_k} \quad \text{as } y \rightarrow 0+, \tag{1.1}$$

where σ_k are known scalars satisfying

$$\sigma_k \neq 0, \quad k = 1, 2, \dots; \quad \Re\sigma_1 < \Re\sigma_2 < \dots; \quad \lim_{k \rightarrow \infty} \Re\sigma_k = +\infty, \tag{1.2}$$

and A and $\alpha_k, k = 1, 2, \dots$, are constants independent of y that are not necessarily known.

From (1.1) and (1.2) it is clear that $A = \lim_{y \rightarrow 0+} A(y)$ when this limit exists. When $\lim_{y \rightarrow 0+} A(y)$ does not exist, A is the antilimit of $A(y)$ for $y \rightarrow 0+$, and in this case $\Re \sigma_1 \leq 0$ necessarily. In any case, A can be approximated very effectively by the Richardson extrapolation process that is defined via the linear systems of equations

$$A(y_l) = A_n^{(j)} + \sum_{k=1}^n \bar{\alpha}_k y_l^{\sigma_k}, \quad j \leq l \leq j + n, \tag{1.3}$$

with the y_l picked as

$$y_l = y_0 \omega^l, \quad l = 0, 1, \dots, \quad \text{for some } y_0 \in (0, b] \text{ and } \omega \in (0, 1). \tag{1.4}$$

Here $A_n^{(j)}$ are the approximations to A and the $\bar{\alpha}_k$ are additional (auxiliary) unknowns. As is well known, $A_n^{(j)}$ can be computed very efficiently by the following algorithm due to Bulirsch and Stoer [2]:

$$\begin{aligned} A_0^{(j)} &= A(y_j), \quad j = 0, 1, \dots, \\ A_n^{(j)} &= \frac{A_{n-1}^{(j+1)} - c_n A_{n-1}^{(j)}}{1 - c_n}, \quad j = 0, 1, \dots, \quad n = 1, 2, \dots, \end{aligned} \tag{1.5}$$

where we have defined

$$c_n = \omega^{\sigma_n}, \quad n = 1, 2, \dots \tag{1.6}$$

Let us now consider the situation in which $A(y)$ and hence A depend on some real or complex parameter ξ and are continuously differentiable in ξ for ξ in some set X of the real line or the complex plane, and we are interested in computing $(d/d\xi)A \equiv \dot{A}$. Let us assume in addition to the above that $(d/d\xi)A(y) \equiv \dot{A}(y)$ has an asymptotic expansion for $y \rightarrow 0+$ that is obtained by differentiating that in (1.1) term by term. (This assumption is satisfied at least in some cases of practical interest as can be shown rigorously.) Finally, let us assume that the α_k and σ_k , as well as $A(y)$ and A , depend on ξ and that they are continuously differentiable for $\xi \in X$. As a consequence of these assumptions we have

$$\dot{A}(y) \sim \dot{A} + \sum_{k=1}^{\infty} (\dot{\alpha}_k + \alpha_k \dot{\sigma}_k \log y) y^{\sigma_k} \quad \text{as } y \rightarrow 0+, \tag{1.7}$$

where $\dot{\alpha}_k \equiv (d/d\xi)\alpha_k$ and $\dot{\sigma}_k \equiv (d/d\xi)\sigma_k$. Obviously, \dot{A} and the $\dot{\alpha}_k$ and $\dot{\sigma}_k$ are independent of y . As a result, the infinite sum on the right-hand side of (1.7) is simply of the form $\sum_{k=1}^{\infty} (\alpha_{k0} + \alpha_{k1} \log y) y^{\sigma_k}$ with α_{k0} and α_{k1} constants independent of y .

Note that when the σ_k do not depend on ξ , we have $\dot{\sigma}_k = 0$ for all k , and, therefore, the asymptotic expansion in (1.7) becomes of exactly the same form as that given in (1.1). This means that we can apply the Richardson extrapolation process above directly to $\dot{A}(y)$ and obtain very good approximations to \dot{A} . This amounts to replacing $A(y_j)$ in (1.5) by $\dot{A}(y_j)$, keeping everything else the same. However, when the σ_k are functions of ξ , the asymptotic expansion in (1.7) is essentially different from that in (1.1). This is so since $y^{\sigma_k} \log y$ and y^{σ_k} behave entirely differently as $y \rightarrow 0+$. In this case the application of the Richardson extrapolation process directly to $\dot{A}(y)$ does not produce approximations to \dot{A} that are of practical value.

The existence of an asymptotic expansion for $\dot{A}(y)$ of the form given in (1.7), however, suggests immediately that a generalized Richardson extrapolation process can be applied to produce approximations to \dot{A} in an efficient manner. In keeping with the convention introduced by the author in [12], this extrapolation process is defined via the linear systems

$$B(y_l) = B_n^{(j)} + \sum_{k=1}^{\lfloor (n+1)/2 \rfloor} \bar{\alpha}_{k0} y_l^{\sigma_k} + \sum_{k=1}^{\lfloor n/2 \rfloor} \bar{\alpha}_{k1} y_l^{\sigma_k} \log y_l, \quad j \leq l \leq j + n, \tag{1.8}$$

where $B(y) \equiv \dot{A}(y)$, $B_n^{(j)}$ are the approximations to $B \equiv \dot{A}$, and $\bar{\alpha}_{k0}$ and $\bar{\alpha}_{k1}$ are additional (auxiliary) unknowns. (This amounts to “eliminating” from (1.7) the functions y^{σ_1} , $y^{\sigma_1} \log y$, y^{σ_2} , $y^{\sigma_2} \log y$, ..., in this order.) With the y_l as in (1.4), the approximations $B_n^{(j)}$ can be computed very efficiently by the following algorithm developed in Sidi [12] and denoted the SGRom-algorithm there:

$$B_0^{(j)} = B(y_j), \quad j = 0, 1, \dots, \\ B_n^{(j)} = \frac{B_{n-1}^{(j+1)} - \lambda_n B_{n-1}^{(j)}}{1 - \lambda_n}, \quad j = 0, 1, \dots, \quad n = 1, 2, \dots, \tag{1.9}$$

where we have now defined

$$\lambda_{2k-1} = \lambda_{2k} = c_k, \quad k = 1, 2, \dots, \tag{1.10}$$

with the c_n as defined in (1.6).

Before going on, we would like to mention that the problem we have described above arises naturally in the numerical evaluation of integrals of the form $B = \int_0^1 (\log x) x^\xi g(x) dx$, where $\Re \xi > -1$ and $g \in C^\infty[0, 1]$. It is easy to see that $B = (d/d\xi)A$, where $A = \int_0^1 x^\xi g(x) dx$. Furthermore, the trapezoidal rule approximation $B(h)$ to B with stepsize h has an Euler–Maclaurin (E–M) expansion that is obtained by differentiating with respect to ξ the E–M expansion of the trapezoidal rule approximation $A(h)$ to A . With this knowledge available, B can be approximated by applying a generalized Richardson extrapolation process to $B(h)$. Traditionally, this approach has been adopted in multidimensional integration of singular functions as well. For a detailed discussion see [3,9].

If we arrange the $A_n^{(j)}$ and $B_n^{(j)}$ in two-dimensional arrays of the form

$$\begin{matrix} Q_0^{(0)} \\ Q_0^{(1)} & Q_1^{(0)} \\ Q_0^{(2)} & Q_1^{(1)} & Q_2^{(0)} \\ Q_0^{(3)} & Q_1^{(2)} & Q_2^{(1)} & Q_3^{(0)} \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{matrix} \tag{1.11}$$

then the diagonal sequences $\{Q_n^{(j)}\}_{n=0}^\infty$ with fixed j have much better convergence properties than the column sequences $\{Q_n^{(j)}\}_{j=0}^\infty$ with fixed n . In particular, the following convergence results are

known:

1. The column sequences satisfy

$$\begin{aligned}
 A_n^{(j)} - A &= O(|c_{n+1}|^j) \quad \text{as } j \rightarrow \infty, \\
 B_{2m+s}^{(j)} - B &= O(j^{1-s}|c_{m+1}|^j) \quad \text{as } j \rightarrow \infty, \quad s = 0, 1.
 \end{aligned}
 \tag{1.12}$$

2. Under the additional condition that

$$\Re\sigma_{k+1} - \Re\sigma_k \geq d > 0, \quad k = 1, 2, \dots, \quad \text{for some fixed } d
 \tag{1.13}$$

and assuming that α_k , $\dot{\alpha}_k$, and $\alpha_k \dot{\sigma}_k$ grow with k at most like $\exp(\beta k^n)$ for some $\beta \geq 0$ and $\eta < 2$, the diagonal sequences satisfy, for all practical purposes,

$$\begin{aligned}
 A_n^{(j)} - A &\doteq O\left(\prod_{i=1}^n |c_i|\right) \quad \text{as } n \rightarrow \infty, \\
 B_n^{(j)} - B &\doteq O\left(\prod_{i=1}^n |\lambda_i|\right) \quad \text{as } n \rightarrow \infty.
 \end{aligned}
 \tag{1.14}$$

The results pertaining to $A_n^{(j)}$ in (1.12) and (1.14), with real σ_k , are due to Bulirsch and Stoer [2]. The case of complex σ_k is contained in [12], and so are the results on $B_n^{(j)}$. Actually, [12] gives a complete treatment of the general case in which

$$A(y) \sim A + \sum_{k=1}^{\infty} \left[\sum_{i=0}^{q_k} \alpha_{ki} (\log y)^i \right] y^{\sigma_k} \quad \text{as } y \rightarrow 0+,
 \tag{1.15}$$

where q_k are known arbitrary nonnegative integers, and α_{ki} are constants independent of y , and the σ_k satisfy the condition

$$\sigma_k \neq 0, \quad k = 1, 2, \dots, \quad \Re\sigma_1 \leq \Re\sigma_2 \leq \dots, \quad \lim_{k \rightarrow \infty} \Re\sigma_k = +\infty
 \tag{1.16}$$

that is much weaker than that in (1.2). Thus, the asymptotic expansions in (1.1) and (1.7) are special cases of that in (1.15) with $q_k = 0$, $k = 1, 2, \dots$, and $q_k = 1$, $k = 1, 2, \dots$, respectively.

Comparison of the diagonal sequences $\{A_n^{(j)}\}_{n=0}^{\infty}$ and $\{B_n^{(j)}\}_{n=0}^{\infty}$ (with j fixed) with the help of (1.14) reveals that the latter has inferior convergence properties, even though the computational costs of $A_n^{(j)}$ and $B_n^{(j)}$ are almost identical. (They involve the computation of $A(y_l)$, $j \leq l \leq j+n$, and $B(y_l)$, $j \leq l \leq j+n$, respectively). As a matter of fact, from (1.6), (1.10), and (1.13) it follows that the bound on $|A_{2m}^{(j)} - A|$ is smaller than that of $|B_{2m}^{(j)} - B|$ by a factor of $O(\prod_{i=1}^m |c_{m+i}/c_i|) = O(\omega^{dm^2})$ as $m \rightarrow \infty$. This theoretical observation is also supported by numerical experiments. Judging from (1.14) again, we see that, when $\Re\sigma_{k+1} - \Re\sigma_k = d$ for all k in (1.13), $B_{\lfloor \sqrt{2} n \rfloor}^{(j)}$ will have an accuracy comparable to that of $A_n^{(j)}$. This, however, increases the cost of the extrapolation substantially, as the cost of computing $A(y_l)$ and $B(y_l)$ increases drastically with increasing l in most cases of interest. This quantitative discussion makes it clear that the inferiority of $B_n^{(j)}$ relative to $A_n^{(j)}$ is actually mathematical and has nothing to do with numerics.

From what we have so far it is easy to identify the Richardson extrapolation of (1.3) as method E_0 and the generalized Richardson extrapolation of (1.8) as method E_1 . We now turn to the new procedure “ $(d/d\xi)E_0$ ”.

Let us now approximate \dot{A} by $(d/d\xi)A_n^{(j)} = \dot{A}_n^{(j)}$. This can be achieved computationally by differentiating the recursion relation in (1.5), the result being the following recursive algorithm:

$$\begin{aligned}
 A_0^{(j)} &= A(y_j) \quad \text{and} \quad \dot{A}_0^{(j)} = \dot{A}(y_j), \quad j = 0, 1, \dots, \\
 A_n^{(j)} &= \frac{A_{n-1}^{(j+1)} - c_n A_{n-1}^{(j)}}{1 - c_n} \quad \text{and} \\
 \dot{A}_n^{(j)} &= \frac{\dot{A}_{n-1}^{(j+1)} - c_n \dot{A}_{n-1}^{(j)}}{1 - c_n} + \frac{\dot{c}_n}{1 - c_n} (A_n^{(j)} - A_{n-1}^{(j)}), \quad j = 0, 1, \dots, \quad n = 1, 2, \dots \quad (1.17)
 \end{aligned}$$

Here $\dot{c}_n \equiv (d/d\xi)c_n$, $n = 1, 2, \dots$. This shows that we need two tables of the form given in (1.11), one for $A_n^{(j)}$ and another for $\dot{A}_n^{(j)}$. We also see that the computation of the $\dot{A}_n^{(j)}$ involves both $\dot{A}(y)$ and $A(y)$.

The column sequences $\{\dot{A}_n^{(j)}\}_{j=0}^\infty$ converge to \dot{A} almost in the same way the corresponding sequences $\{A_n^{(j)}\}_{j=0}^\infty$ converge to A , cf. (1.12). We have

$$\dot{A}_n^{(j)} - \dot{A} = O(j|c_{n+1}|^j) \quad \text{as } j \rightarrow \infty. \quad (1.18)$$

The diagonal sequences $\{\dot{A}_n^{(j)}\}_{n=0}^\infty$ converge to \dot{A} also practically the same way the corresponding $\{A_n^{(j)}\}_{n=0}^\infty$ converge to A , subject to the mild conditions that $\sum_{i=1}^\infty |\dot{c}_i| < \infty$ and $\sum_{i=1}^n |\dot{c}_i/c_i| = O(n^a)$ as $n \rightarrow \infty$ for some $a \geq 0$, in addition to (1.13). We have for all practical purposes, cf. (1.14),

$$\dot{A}_n^{(j)} - \dot{A} \doteq O\left(\prod_{i=1}^n |c_i|\right) \quad \text{as } n \rightarrow \infty. \quad (1.19)$$

The stability properties of the column and diagonal sequences of the $\dot{A}_n^{(j)}$ are likewise analyzed in [14] and are shown to be very similar to those of the $A_n^{(j)}$. We refer the reader to [14] for details.

This completes our review of the motivation and results of [14]. In the next section we present the extension of the procedure of [14] to GREP⁽¹⁾. We derive the recursive algorithm for computing the approximations and for assessing their numerical stability. In Section 3 we discuss the stability and convergence properties of the new procedure subject to a set of appropriate sufficient conditions that are met in many cases of interest. The main results of this section are Theorem 3.3 on stability and Theorem 3.4 on convergence and both are optimal asymptotically. In Section 4 we show how the method and theory of Sections 2 and 3 apply to the summation of some infinite series of logarithmic type via the $d^{(1)}$ -transformation. Finally, in Section 5 we give two numerical examples that illustrate the theory and show the superiority of the new approach to derivatives of limits over the direct one. In the first example we apply the new approach to the computation of the derivative of the Riemann zeta function. In the second example we compute $(d/d\xi)F(\xi, \frac{1}{2}; \frac{3}{2}; 1)$, where $F(a, b; c; z)$ is

the Gauss hypergeometric function. This example shows clearly that our approach is very effective for computing derivatives of special functions such as the hypergeometric functions with respect to their parameters.

2. GREP⁽¹⁾ and its derivative

2.1. General preliminaries on GREP⁽¹⁾

As GREP⁽¹⁾ applies to functions $A(y)$ that are in the class $F^{(1)}$, we start by describing $F^{(1)}$.

Definition 2.1. We shall say that a function $A(y)$, defined for $0 < y \leq b$, for some $b > 0$, where y can be a discrete or continuous variable, belongs to the set $F^{(1)}$, if there exist functions $\phi(y)$ and $\beta(y)$ and a constant A , such that

$$A(y) = A + \phi(y)\beta(y), \tag{2.1}$$

where $\beta(x)$, as a function of the continuous variable x and for some $\eta \leq b$, is continuous for $0 \leq x \leq \eta$, and, for some constant $r > 0$, has a Poincaré-type asymptotic expansion of the form

$$\beta(x) \sim \sum_{i=0}^{\infty} \beta_i x^{ir} \quad \text{as } x \rightarrow 0+. \tag{2.2}$$

If, in addition, the function $B(t) \equiv \beta(t^{1/r})$, as a function of the continuous variable t , is infinitely differentiable for $0 \leq t \leq \eta^r$, we shall say that $A(y)$ belongs to the set $F_{\infty}^{(1)}$. Note that $F_{\infty}^{(1)} \subset F^{(1)}$.

Remark. $A = \lim_{y \rightarrow 0+} A(y)$ whenever this limit exists. If $\lim_{y \rightarrow 0+} A(y)$ does not exist, then A is said to be the antilimit of $A(y)$. In this case $\lim_{y \rightarrow 0+} \phi(y)$ does not exist as is obvious from (2.1) and (2.2).

It is assumed that the functions $A(y)$ and $\phi(y)$ are computable for $0 < y \leq b$ (keeping in mind that y may be discrete or continuous depending on the situation) and that the constant r is known. The constants A and β_i are not assumed to be known. The problem is to find (or approximate) A whether it is the limit or the antilimit of $A(y)$ as $y \rightarrow 0+$, and GREP⁽¹⁾, the extrapolation procedure that corresponds to $F^{(1)}$, is designed to tackle precisely this problem.

Definition 2.2. Let $A(y) \in F^{(1)}$, with $\phi(y)$, $\beta(y)$, A , and r being exactly as in Definition 2.1. Pick $y_l \in (0, b]$, $l = 0, 1, 2, \dots$, such that $y_0 > y_1 > y_2 > \dots$, and $\lim_{l \rightarrow \infty} y_l = 0$. Then $A_n^{(j)}$, the approximation to A , and the parameters $\tilde{\beta}_i$, $i = 0, 1, \dots, n - 1$, are defined to be the solution of the system of $n + 1$ linear equations

$$A_n^{(j)} = A(y_l) + \phi(y_l) \sum_{i=0}^{n-1} \tilde{\beta}_i y_l^{ir}, \quad j \leq l \leq j + n, \tag{2.3}$$

provided the matrix of this system is nonsingular. It is this process that generates the approximations $A_n^{(j)}$ that we call GREP⁽¹⁾.

As is seen, GREP⁽¹⁾ produces a two-dimensional table of approximations of the form given in (1.1).

Before going on we let $t = y^r$ and $t_l = y_l^r$, $l = 0, 1, \dots$, and define $a(t) \equiv A(y)$ and $\varphi(t) \equiv \phi(y)$. Then the equations in (2.3) take on the more convenient form

$$A_n^{(j)} = a(t_l) + \varphi(t_l) \sum_{i=0}^{n-1} \tilde{\beta}_i t_l^i, \quad j \leq l \leq j + n. \tag{2.4}$$

A closed-form expression for $A_n^{(j)}$ can be obtained by using divided differences. In the sequel we denote by $D_k^{(s)}$ the divided difference operator of order k over the set of points $t_s, t_{s+1}, \dots, t_{s+k}$. Thus, for any function $g(t)$ defined at these points we have

$$D_k^{(s)}\{g(t)\} = g[t_s, t_{s+1}, \dots, t_{s+k}] = \sum_{l=s}^{s+k} \left(\prod_{\substack{i=s \\ i \neq l}}^{s+k} \frac{1}{t_l - t_i} \right) g(t_l) \equiv \sum_{i=0}^k c_{ki}^{(s)} g(t_{s+i}). \tag{2.5}$$

Then $A_n^{(j)}$ is given by

$$A_n^{(j)} = \frac{D_n^{(j)}\{a(t)/\varphi(t)\}}{D_n^{(j)}\{1/\varphi(t)\}}. \tag{2.6}$$

As is clear from (2.6), $A_n^{(j)}$ can be expressed also in the form

$$A_n^{(j)} = \sum_{i=0}^n \gamma_{ni}^{(j)} a(t_{j+i}), \tag{2.7}$$

where $\gamma_{ni}^{(j)}$ are constants that are independent of $a(t)$ and that depend solely on the t_l and $\varphi(t_l)$ and satisfy $\sum_{i=0}^n \gamma_{ni}^{(j)} = 1$. The quantity $\Gamma_n^{(j)}$ defined by

$$\Gamma_n^{(j)} = \sum_{i=0}^n |\gamma_{ni}^{(j)}| \tag{2.8}$$

(note that $\Gamma_n^{(j)} \geq 1$) plays an important role in assessing the stability properties of the approximation $A_n^{(j)}$ with respect to errors (roundoff or other) in the $a(t_l)$. As has been noted in various places, if ε_l is the (absolute) error committed in the computation of $a(t_l)$, $l = 0, 1, \dots$, then $|A_n^{(j)} - \tilde{A}_n^{(j)}| \leq \Gamma_n^{(j)} (\max_{j \leq l \leq j+n} |\varepsilon_l|)$, where $\tilde{A}_n^{(j)}$ is the computed (as opposed to exact) value of $A_n^{(j)}$. Concerning $\Gamma_n^{(j)}$ we have a result analogous to (2.6), namely,

$$\Gamma_n^{(j)} = \sum_{i=0}^n |\gamma_{ni}^{(j)}| = \frac{|D_n^{(j)}\{u(t)\}|}{|D_n^{(j)}\{1/\varphi(t)\}|}, \tag{2.9}$$

where $u(t)$ is arbitrarily defined for all t except for t_0, t_1, \dots , where it is defined by

$$u(t_l) = (-1)^l / |\varphi(t_l)|, \quad l = 0, 1, \dots \tag{2.10}$$

This is a result of the following lemma that will be used again later in this paper.

Lemma 2.1. With $D_k^{(s)}\{g(t)\}$ as in (2.5), we have

$$\sum_{i=0}^k |c_{ki}^{(s)}| h_{s+i} = (-1)^s D_k^{(s)}\{u(t)\}, \tag{2.11}$$

where h_l are arbitrary scalars and

$$u(t_l) = (-1)^l h_l, \quad l = 0, 1, \dots, \tag{2.12}$$

but $u(t)$ is arbitrary otherwise.

Proof. The validity of (2.11) follows from (2.5) and from the fact that $c_{ki}^{(s)} = (-1)^i |c_{ki}^{(s)}|$, $i=0, 1, \dots, k$. □

The results in (2.6) and (2.9) form the basis of the W -algorithm that is used in computing both the $A_n^{(j)}$ and the $\Gamma_n^{(j)}$ in a very efficient way. For this we define for all j and n

$$M_n^{(j)} = D_n^{(j)}\{a(t)/\varphi(t)\}, \quad N_n^{(j)} = D_n^{(j)}\{1/\varphi(t)\} \quad \text{and} \quad H_n^{(j)} = D_n^{(j)}\{u(t)\} \tag{2.13}$$

with $u(t_l)$ as in (2.10), and recall the well-known recursion relation for divided differences, namely,

$$D_n^{(j)}\{g(t)\} = \frac{D_{n-1}^{(j+1)}\{g(t)\} - D_{n-1}^{(j)}\{g(t)\}}{t_{j+n} - t_j}. \tag{2.14}$$

(See, e.g., [15, p. 45].) Here are the steps of the W -Algorithm:

1. For $j = 0, 1, \dots$, set

$$M_0^{(j)} = a(t_j)/\varphi(t_j), \quad N_0^{(j)} = 1/\varphi(t_j) \quad \text{and} \quad H_0^{(j)} = (-1)^j / |\varphi(t_j)|. \tag{2.15}$$

2. For $j = 0, 1, \dots$, and $n = 1, 2, \dots$, compute $M_n^{(j)}$, $N_n^{(j)}$, and $H_n^{(j)}$ recursively from

$$Q_n^{(j)} = \frac{Q_{n-1}^{(j+1)} - Q_{n-1}^{(j)}}{t_{j+n} - t_j} \tag{2.16}$$

with $Q_n^{(j)}$ equal to $M_n^{(j)}$, $N_n^{(j)}$, and $H_n^{(j)}$.

3. For all j and n set

$$A_n^{(j)} = \frac{M_n^{(j)}}{N_n^{(j)}} \quad \text{and} \quad \Gamma_n^{(j)} = \frac{|H_n^{(j)}|}{|N_n^{(j)}|}. \tag{2.17}$$

Note that the W -Algorithm for $A_n^{(j)}$ was originally developed in [8]. The recursion for $\Gamma_n^{(j)}$ was given recently in [10]. Stability and convergence studies for GREP⁽¹⁾ can be found in [10], and more recently in [13].

Let us now assume that $A(y)$ and A depend on a real or complex parameter ξ and that we would like to compute $(d/d\xi)A \equiv \dot{A}$ assuming that \dot{A} is the limit or antilimit of $(d/d\xi)A(y)$ as $y \rightarrow 0+$. We also assume that $\phi(y)$ and β_i in (2.1) are differentiable functions of ξ and that $\dot{A}(y)$ has an asymptotic expansion as $y \rightarrow 0+$ obtained by differentiating that of $A(y)$ given in (2.1) and (2.2) term by term. Thus

$$\dot{A}(y) \sim \dot{A} + \dot{\phi}(y) \sum_{i=0}^{\infty} \beta_i y^{ir} + \phi(y) \sum_{i=0}^{\infty} \dot{\beta}_i y^{ir} \quad \text{as } y \rightarrow 0+. \tag{2.18}$$

Here $\dot{\phi}(y) \equiv (d/d\xi)\phi(y)$ and $\dot{\beta}_i \equiv (d/d\xi)\beta_i$ in keeping with the convention of the previous section.

We can now approximate \dot{A} by applying the extrapolation process GREP⁽²⁾ to (2.18). The approximations $B_n^{(j)}$ to $B \equiv \dot{A}$ that result from this are defined via the linear systems

$$B(y_l) = B_n^{(j)} + \phi(y_l) \sum_{i=0}^{\lfloor (n-1)/2 \rfloor} \bar{\beta}_{1i} y_l^{ir} + \dot{\phi}(y_l) \sum_{i=0}^{\lfloor n/2 \rfloor - 1} \bar{\beta}_{2i} y_l^{ir}, \quad j \leq l \leq j+n, \tag{2.19}$$

where $B(y) \equiv \dot{A}(y)$ as before. (Compare (2.18) and (2.19) with (1.7) and (1.8), respectively.) Now the $B_n^{(j)}$ converge to \dot{A} , but their rate of convergence to \dot{A} is inferior to that of the corresponding $A_n^{(j)}$ to A . We, therefore, would like to employ the approach of [14] hoping that it will produce better results also with GREP⁽¹⁾.

2.2. (d/dξ)GREP⁽¹⁾ and its implementation

Let us differentiate (2.7) with respect to ξ . We obtain

$$\dot{A}_n^{(j)} = \sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} \dot{a}(t_{j+i}) + \sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} a(t_{j+i}), \tag{2.20}$$

where $\dot{\gamma}_{ni}^{(j)} \equiv (d/d\xi)\gamma_{ni}^{(j)}$ and $\dot{a}(t) \equiv (d/d\xi)a(t) \equiv \dot{A}(y)$.

It is clear that, unlike $B_n^{(j)}$ in (2.19) that depends only on $\dot{a}(t)$, $\dot{A}_n^{(j)}$ depends on both $\dot{a}(t)$ and $a(t)$. Also the stability of $\dot{A}_n^{(j)}$ is affected by errors both in $a(t_l)$ and $\dot{a}(t_l)$. In particular, if ε_l and η_l are the (absolute) errors in $a(t_l)$ and $\dot{a}(t_l)$, respectively, then $|\dot{A}_n^{(j)} - \bar{\dot{A}}_n^{(j)}| \leq \Omega_n^{(j)} [\max_{j \leq l \leq j+n} \max(|\varepsilon_l|, |\eta_l|)]$, where $\bar{\dot{A}}_n^{(j)}$ is the computed (as opposed to exact) value of $\dot{A}_n^{(j)}$, and

$$\Omega_n^{(j)} = \sum_{i=0}^n |\dot{\gamma}_{ni}^{(j)}| + \sum_{i=0}^n |\gamma_{ni}^{(j)}|. \tag{2.21}$$

We shall call this extension of GREP⁽¹⁾ simply (d/dξ)GREP⁽¹⁾.

2.2.1. Computation of $\dot{A}_n^{(j)}$

Let us start by differentiating $A_n^{(j)} = M_n^{(j)} / N_n^{(j)}$. Upon denoting $(d/d\xi)M_n^{(j)} = \dot{M}_n^{(j)}$ and $(d/d\xi)N_n^{(j)} = \dot{N}_n^{(j)}$, we have

$$\dot{A}_n^{(j)} = \frac{\dot{M}_n^{(j)}}{N_n^{(j)}} - \frac{M_n^{(j)} \dot{N}_n^{(j)}}{[N_n^{(j)}]^2}. \tag{2.22}$$

Now $M_n^{(j)}$ and $N_n^{(j)}$ are already available from the W -algorithm. We need only compute $\dot{M}_n^{(j)}$ and $\dot{N}_n^{(j)}$, and these can be computed by direct differentiation of (2.16) along with the appropriate initial conditions in (2.15).

2.2.2. Computation of an upper bound on $\Omega_n^{(j)}$

The assessment of stability of $\dot{A}_n^{(j)}$ turns out to be much more involved than that of $A_n^{(j)}$, and it requires a good understanding of the nature of $\dot{M}_n^{(j)}$.

First, we note that, as the t_l are independent of ζ , $D_n^{(j)}$ and $(d/d\zeta)$ commute, i.e., $(d/d\zeta)D_n^{(j)}\{g(t)\} = D_n^{(j)}\{(d/d\zeta)g(t)\}$. Consequently, from (2.16) we have

$$\dot{M}_n^{(j)} = D_n^{(j)} \left\{ \frac{d}{d\zeta} \frac{a(t)}{\varphi(t)} \right\} = D_n^{(j)} \left\{ \frac{\dot{a}(t)}{\varphi(t)} - \frac{a(t)\dot{\varphi}(t)}{[\varphi(t)]^2} \right\}. \tag{2.23}$$

Next, substituting (2.23) in (2.22), and using the fact that $D_n^{(j)}$ is a linear operator, we obtain

$$\dot{A}_n^{(j)} = Y_1 + Y_2 + Y_3, \tag{2.24}$$

where

$$\begin{aligned} Y_1 &= \frac{D_n^{(j)}\{\dot{a}(t)/\varphi(t)\}}{N_n^{(j)}} = \sum_{i=0}^n \gamma_{ni}^{(j)} \dot{a}(t_{j+i}), \\ Y_2 &= -\frac{\dot{N}_n^{(j)} D_n^{(j)}\{a(t)/\varphi(t)\}}{[N_n^{(j)}]^2} = -\frac{\dot{N}_n^{(j)}}{N_n^{(j)}} \sum_{i=0}^n \gamma_{ni}^{(j)} a(t_{j+i}), \\ Y_3 &= -\frac{D_n^{(j)}\{a(t)\dot{\varphi}(t)/[\varphi(t)]^2\}}{N_n^{(j)}} = -\sum_{i=0}^n \delta_{ni}^{(j)} a(t_{j+i}) \end{aligned} \tag{2.25}$$

with $\delta_{ni}^{(j)} = \gamma_{ni}^{(j)} \dot{\varphi}(t_{j+i})/\varphi(t_{j+i})$. Here we have used the fact that

$$\frac{D_n^{(j)}\{h(t)/\varphi(t)\}}{D_n^{(j)}\{1/\varphi(t)\}} = \sum_{i=0}^n \gamma_{ni}^{(j)} h(t_{j+i}) \quad \text{for any } h(t). \tag{2.26}$$

Recalling (2.20), we identify

$$\dot{\gamma}_{ni}^{(j)} = -\frac{\dot{N}_n^{(j)}}{N_n^{(j)}} \gamma_{ni}^{(j)} - \delta_{ni}^{(j)}, \quad i = 0, 1, \dots, n. \tag{2.27}$$

Therefore,

$$\Omega_n^{(j)} = \sum_{i=0}^n |\gamma_{ni}^{(j)}| + \sum_{i=0}^n \left| \frac{\dot{N}_n^{(j)}}{N_n^{(j)}} \gamma_{ni}^{(j)} + \delta_{ni}^{(j)} \right| = \sum_{i=0}^n |\gamma_{ni}^{(j)}| + \sum_{i=0}^n |\gamma_{ni}^{(j)}| \left| \frac{\dot{N}_n^{(j)}}{N_n^{(j)}} + \frac{\dot{\varphi}(t_{j+i})}{\varphi(t_{j+i})} \right|. \tag{2.28}$$

Now even though the first summation is simply $\Gamma_n^{(j)}$, and hence can be computed very inexpensively, the second sum cannot, as its general term depends also on $\dot{N}_n^{(j)}/N_n^{(j)}$, hence on j and n . We can, however, compute, again very inexpensively, an upper bound $\tilde{\Omega}_n^{(j)}$ on $\Omega_n^{(j)}$, defined by

$$\tilde{\Omega}_n^{(j)} = \Gamma_n^{(j)} + \frac{|\dot{N}_n^{(j)}|}{|N_n^{(j)}|} \Gamma_n^{(j)} + \Theta_n^{(j)} \quad \text{where } \Theta_n^{(j)} \equiv \sum_{i=0}^n |\delta_{ni}^{(j)}| \tag{2.29}$$

which is obtained by manipulating the second summation in (2.28) appropriately. This can be achieved by first realizing that

$$\Theta_n^{(j)} = \frac{|D_n^{(j)}\{v(t)\}|}{|N_n^{(j)}|}, \tag{2.30}$$

where $v(t)$ is arbitrarily defined for all t except for t_0, t_1, \dots , for which it is defined by

$$v(t_l) = (-1)^l |\dot{\varphi}(t_l)| / |\varphi(t_l)|^2, \quad l = 0, 1, \dots \tag{2.31}$$

and then by applying Lemma 2.1.

2.2.3. The (d/dξ)W-algorithm for $\dot{A}_n^{(j)}$

Combining all of the developments above, we can now extend the W -algorithm to compute $\dot{A}_n^{(j)}$ and $\tilde{\Omega}_n^{(j)}$. We shall denote the resulting algorithm the (d/dξ)W-algorithm. Here are the steps of this algorithm.

1. For $j = 0, 1, \dots$, set

$$M_0^{(j)} = \frac{a(t_j)}{\varphi(t_j)}, \quad N_0^{(j)} = \frac{1}{\varphi(t_j)}, \quad H_0^{(j)} = (-1)^j |N_0^{(j)}|, \quad \text{and}$$

$$\dot{M}_0^{(j)} = \frac{\dot{a}(t_j)}{\varphi(t_j)} - \frac{a(t_j)\dot{\varphi}(t_j)}{[\varphi(t_j)]^2}, \quad \dot{N}_0^{(j)} = -\frac{\dot{\varphi}(t_j)}{[\varphi(t_j)]^2}, \quad \tilde{H}_0^{(j)} = (-1)^j |\dot{N}_0^{(j)}|. \tag{2.32}$$

2. For $j=0, 1, \dots$, and $n=1, 2, \dots$, compute $M_n^{(j)}$, $N_n^{(j)}$, $H_n^{(j)}$, $\dot{M}_n^{(j)}$, $\dot{N}_n^{(j)}$, and $\tilde{H}_n^{(j)}$ recursively from

$$Q_n^{(j)} = \frac{Q_{n-1}^{(j+1)} - Q_{n-1}^{(j)}}{t_{j+n} - t_j}. \tag{2.33}$$

3. For all j and n set

$$A_n^{(j)} = \frac{M_n^{(j)}}{N_n^{(j)}}, \quad \Gamma_n^{(j)} = \frac{|H_n^{(j)}|}{|N_n^{(j)}|}, \quad \text{and}$$

$$\dot{A}_n^{(j)} = \frac{\dot{M}_n^{(j)}}{N_n^{(j)}} - A_n^{(j)} \frac{\dot{N}_n^{(j)}}{N_n^{(j)}}, \quad \tilde{\Omega}_n^{(j)} = \frac{|\tilde{H}_n^{(j)}|}{|N_n^{(j)}|} + \left(1 + \frac{|\dot{N}_n^{(j)}|}{|N_n^{(j)}|} \right) \Gamma_n^{(j)}. \tag{2.34}$$

It is interesting to note that we need six tables of the form (1.11) in order to carry out the (d/dξ)W-algorithm. This is *twice* the number of tables needed to carry out the W -algorithm. Note also that no tables need to be saved for $A_n^{(j)}$, $\Gamma_n^{(j)}$, $\dot{A}_n^{(j)}$, and $\tilde{\Omega}_n^{(j)}$. This seems to be the situation for all extrapolation methods.

3. Column convergence for (d/dξ)GREP⁽¹⁾

In this section we shall give a detailed analysis of the column sequences $\{\dot{A}_n^{(j)}\}_{j=0}^\infty$ with n fixed for the case in which the t_l are picked such that

$$t_0 > t_1 > \dots > 0 \quad \text{and} \quad \lim_{m \rightarrow \infty} \frac{t_{m+1}}{t_m} = \omega \quad \text{for some } \omega \in (0, 1). \tag{3.1}$$

We also assume that

$$\lim_{m \rightarrow \infty} \frac{\varphi(t_{m+1})}{\varphi(t_m)} = \omega^\delta \quad \text{for some (complex) } \delta \neq 0, -1, -2, \dots \tag{3.2}$$

Recalling from Definition 2.1 that $\beta(y) \equiv B(t) \sim \sum_{i=0}^\infty \beta_i t^i$ as $t \rightarrow 0+$, we already have the following optimal convergence and stability results for $A_n^{(j)}$ and $\Gamma_n^{(j)}$, see Theorems 2.1 and 2.2 in [10].

Theorem 3.1. *Under the conditions given in (3.1) and (3.2), we have*

$$A_n^{(j)} - A \sim \left(\prod_{i=1}^n \frac{c_{n+\mu+1} - c_i}{1 - c_i} \right) \beta_{n+\mu} \varphi(t_j) t_j^{n+\mu} \quad \text{as } j \rightarrow \infty, \tag{3.3}$$

where $\beta_{n+\mu}$ is the first nonzero β_i with $i \geq n$, and

$$\lim_{j \rightarrow \infty} \sum_{i=0}^n \gamma_{ni}^{(j)} z^i = \prod_{i=1}^n \frac{z - c_i}{1 - c_i} \equiv U_n(z) \equiv \sum_{i=0}^n \tilde{\gamma}_{ni} z^i, \tag{3.4}$$

so that for each fixed n

$$\lim_{j \rightarrow \infty} \Gamma_n^{(j)} = \prod_{i=1}^n \frac{1 + |c_i|}{|1 - c_i|} \quad \text{hence} \quad \sup_j \Gamma_n^{(j)} < \infty. \tag{3.5}$$

Here

$$c_k = \omega^{\delta+k-1}, \quad k = 1, 2, \dots \tag{3.6}$$

We shall see below that what we need for the analysis of (d/dξ)GREP⁽¹⁾ are the asymptotic behaviors of $\gamma_{ni}^{(j)}$ and $\tilde{\gamma}_{ni}^{(j)}$. Now that we know the behavior of $\gamma_{ni}^{(j)}$ as $j \rightarrow \infty$ from (3.4), we turn to the study of $\tilde{\gamma}_{ni}^{(j)}$. We start with

$$\sum_{i=0}^n \tilde{\gamma}_{ni}^{(j)} z^i = \frac{T_n^{(j)}(z)}{T_n^{(j)}(1)} \quad \text{with} \quad T_n^{(j)}(z) = \sum_{i=0}^n \frac{c_{ni}^{(j)}}{\varphi(t_{j+i})} z^i, \tag{3.7}$$

which follows from the fact that $\gamma_{ni}^{(j)} = [c_{ni}^{(j)} / \varphi(t_{j+i})] / D_n^{(j)}\{1/\varphi(t)\}$. Of course, $T_n^{(j)}(1) = D_n^{(j)}\{1/\varphi(t)\}$.

Differentiating (3.7) with respect to ξ , and denoting $\dot{T}_n^{(j)}(z) = (d/d\xi)T_n^{(j)}(z)$, we obtain

$$\sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} z^i = \frac{\dot{T}_n^{(j)}(z)T_n^{(j)}(1) - T_n^{(j)}(z)\dot{T}_n^{(j)}(1)}{[T_n^{(j)}(1)]^2}. \tag{3.8}$$

Obviously,

$$\dot{T}_n^{(j)}(z) = - \sum_{i=0}^n c_{ni}^{(j)} \frac{\dot{\phi}(t_{j+i})}{[\phi(t_{j+i})]^2} z^i, \tag{3.9}$$

as a result of which we have

$$\frac{\dot{T}_n^{(j)}(z)}{T_n^{(j)}(1)} = - \sum_{i=0}^n \gamma_{ni}^{(j)} \frac{\dot{\phi}(t_{j+i})}{\phi(t_{j+i})} z^i. \tag{3.10}$$

Substituting (3.10) in (3.8) and using the fact that $\sum_{i=0}^n \gamma_{ni}^{(j)} = 1$, we finally get

$$\sum_{i=0}^n \gamma_{ni}^{(j)} z^i = - \sum_{i=0}^n \gamma_{ni}^{(j)} \frac{\dot{\phi}(t_{j+i})}{\phi(t_{j+i})} z^i + \left(\sum_{i=0}^n \gamma_{ni}^{(j)} z^i \right) \left(\sum_{i=0}^n \gamma_{ni}^{(j)} \frac{\dot{\phi}(t_{j+i})}{\phi(t_{j+i})} \right). \tag{3.11}$$

We have now come to the point where we have to make a suitable assumption on $\dot{\phi}(t)$. The following assumption seems to be quite realistic for many examples that involve logarithmically convergent sequences and some others as well:

$$\dot{\phi}(t) = \phi(t)[K \log t + L + o(1)] \quad \text{as } t \rightarrow 0+ \quad \text{for some constants } K \neq 0 \text{ and } L. \tag{3.12}$$

Now the condition $\lim_{m \rightarrow \infty} (t_{m+1}/t_m) = \omega$ in (3.1) implies that $t_{m+1}/t_m = \omega(1 + \varepsilon_m)$, where $\lim_{m \rightarrow \infty} \varepsilon_m = 0$. Therefore, $t_{j+i} = t_j \omega^i \prod_{s=0}^{i-1} (1 + \varepsilon_{j+s})$, and hence, for each fixed $i \geq 0$

$$\log t_{j+i} = \log t_j + i \log \omega + \varepsilon_i^{(j)}, \quad \lim_{j \rightarrow \infty} \varepsilon_i^{(j)} = 0, \tag{3.13}$$

since $\varepsilon_i^{(j)} = O(\max\{|\varepsilon_j|, |\varepsilon_{j+1}|, \dots, |\varepsilon_{j+1-i}|\})$. Next, (3.12) and (3.13) imply that, for each fixed $i \geq 0$,

$$\frac{\dot{\phi}(t_{j+i})}{\phi(t_{j+i})} = (K \log t_j + L) + Ki \log \omega + \sigma_i^{(j)}, \quad \lim_{j \rightarrow \infty} \sigma_i^{(j)} = 0, \tag{3.14}$$

since $\lim_{m \rightarrow \infty} t_m = 0$.

Substituting (3.14) in (3.11), we see that the problematic term $(K \log t_j + L)$ that is unbounded as $j \rightarrow \infty$ disappears altogether, and we obtain

$$\sum_{i=0}^n \gamma_{ni}^{(j)} z^i = - \sum_{i=0}^n \gamma_{ni}^{(j)} (Ki \log \omega + \sigma_i^{(j)}) z^i + \left(\sum_{i=0}^n \gamma_{ni}^{(j)} z^i \right) \left(\sum_{i=0}^n \gamma_{ni}^{(j)} (Ki \log \omega + \sigma_i^{(j)}) \right). \tag{3.15}$$

Letting $j \rightarrow \infty$ in (3.15) and invoking $\lim_{j \rightarrow \infty} \sigma_i^{(j)} = 0$ and recalling from Theorem 3.1 that $\lim_{j \rightarrow \infty} \gamma_{ni}^{(j)} = \tilde{\gamma}_{ni}$, we obtain the finite limit

$$\lim_{j \rightarrow \infty} \sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} z^i = K \log \omega \left\{ \left(\sum_{i=0}^n \tilde{\gamma}_{ni} z^i \right) \left(\sum_{i=0}^n i \tilde{\gamma}_{ni} \right) - \left(\sum_{i=0}^n i \tilde{\gamma}_{ni} z^i \right) \right\}. \tag{3.16}$$

The following theorem summarizes the developments of this section up to this point.

Theorem 3.2. *Subject to the conditions concerning the t_l and $\varphi(t)$ that are given in (3.1), (3.2), and (3.12), $\sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} z^i$ has a finite limit as $j \rightarrow \infty$ that is given by*

$$\lim_{j \rightarrow \infty} \sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} z^i = K \log \omega [U_n(z)U_n'(1) - zU_n'(z)] \equiv W_n(z) \equiv \sum_{i=0}^n \tilde{\gamma}_{ni} z^i, \tag{3.17}$$

where $U_n(z) = \prod_{i=1}^n \frac{(z-c_i)}{(1-c_i)}$ and $c_i = \omega^{\delta+i-1}$, $i = 1, 2, \dots$, and $U_n'(z) = (d/dz)U_n(z)$.

Theorem 3.2 is the key to the study of stability and convergence of column sequences $\{A_n^{(j)}\}_{j=0}^\infty$ that follows.

3.1. Stability of column sequences $\{A_n^{(j)}\}_{j=0}^\infty$

Theorem 3.3. *Under the conditions of Theorem 3.2, the sequences $\{A_n^{(j)}\}_{j=0}^\infty$ are stable in the sense that $\sup_j \Omega_n^{(j)} < \infty$.*

Proof. The result follows from the facts that $\lim_{j \rightarrow \infty} \gamma_{ni}^{(j)} = \tilde{\gamma}_{ni}$ and $\lim_{j \rightarrow \infty} \dot{\gamma}_{ni}^{(j)} = \tilde{\gamma}_{ni}$ for all n and i , which in turn follow from Theorems 3.1 and 3.2, respectively. \square

3.2. Convergence of column sequences $\{A_n^{(j)}\}_{j=0}^\infty$

Theorem 3.4. *Under the conditions of Theorem 3.2 and with the notation therein we have*

$$\dot{A}_n^{(j)} - \dot{A} = O(\varphi(t_j)t_j^n \log t_j) \quad \text{as } j \rightarrow \infty. \tag{3.18}$$

A more refined result can be stated as follows: If $\beta_{n+\mu}$ is the first nonzero β_i with $i \geq n$ in (2.2) and if β_{n+v} is the first nonzero β_i with $i \geq n$, then

$$\begin{aligned} \dot{A}_n^{(j)} - \dot{A} &= \dot{\beta}_{n+v} U_n(c_{n+v+1}) \varphi(t_j) t_j^{n+v} [1 + o(1)] \\ &\quad + K \beta_{n+\mu} U_n(c_{n+\mu+1}) \varphi(t_j) t_j^{n+\mu} \log t_j [1 + o(1)] \quad \text{as } j \rightarrow \infty. \end{aligned} \tag{3.19}$$

Thus, when $\mu \leq v$ the second term dominates in $\dot{A}_n^{(j)} - \dot{A}$, while the first one does when $\mu > v$. In particular, if $\beta_n \neq 0$, we have

$$\dot{A}_n^{(j)} - \dot{A} \sim K \beta_n U_n(c_{n+1}) \varphi(t_j) t_j^n \log t_j \quad \text{as } j \rightarrow \infty. \tag{3.20}$$

Proof. We start with the fact that

$$A_n^{(j)} - A = \sum_{i=0}^n \gamma_{ni}^{(j)} [a(t_{j+i}) - A] = \sum_{i=0}^n \gamma_{ni}^{(j)} \varphi(t_{j+i}) B_n(t_{j+i}), \tag{3.21}$$

where

$$B_n(t) = B(t) - \sum_{i=0}^{n-1} \beta_i t^i \sim \sum_{i=n}^{\infty} \beta_i t^i \quad \text{as } t \rightarrow 0+. \tag{3.22}$$

Differentiating (3.21) with respect to ξ , we obtain

$$\dot{A}_n^{(j)} - \dot{A} = E_{n,1}^{(j)} + E_{n,2}^{(j)} + E_{n,3}^{(j)} \tag{3.23}$$

with

$$\begin{aligned} E_{n,1}^{(j)} &= \sum_{i=0}^n \dot{\gamma}_{ni}^{(j)} \varphi(t_{j+i}) B_n(t_{j+i}), \\ E_{n,2}^{(j)} &= \sum_{i=0}^n \gamma_{ni}^{(j)} \varphi(t_{j+i}) \dot{B}_n(t_{j+i}), \\ E_{n,3}^{(j)} &= \sum_{i=0}^n \gamma_{ni}^{(j)} \dot{\varphi}(t_{j+i}) B_n(t_{j+i}). \end{aligned} \tag{3.24}$$

By the conditions in (3.1) and (3.2), and by (3.14) that follows from the condition in (3.12), it can be shown that

$$t_{j+i} \sim t_j \omega^i, \quad \varphi(t_{j+i}) \sim \omega^{i\delta} \varphi(t_j), \quad \text{and} \quad \dot{\varphi}(t_{j+i}) \sim K \omega^{i\delta} \varphi(t_j) \log t_j \quad \text{as } j \rightarrow \infty. \tag{3.25}$$

Substituting these in (3.24), noting that $B_n(t) \sim \beta_{n+\mu} t^{n+\mu}$ and $\dot{B}_n(t) \sim \dot{\beta}_{n+\nu} t^{n+\nu}$ as $t \rightarrow 0+$, and recalling (3.4) and (3.17), we obtain

$$\begin{aligned} E_{n,1}^{(j)} &= \beta_{n+\mu} W_n(c_{n+\mu+1}) \varphi(t_j) t_j^{n+\mu} + o(\varphi(t_j) t_j^{n+\mu}) \quad \text{as } j \rightarrow \infty, \\ E_{n,2}^{(j)} &\sim \dot{\beta}_{n+\nu} U_n(c_{n+\nu+1}) \varphi(t_j) t_j^{n+\nu} \quad \text{as } j \rightarrow \infty, \\ E_{n,3}^{(j)} &\sim K \beta_{n+\mu} U_n(c_{n+\mu+1}) \varphi(t_j) t_j^{n+\mu} \log t_j \quad \text{as } j \rightarrow \infty, \end{aligned} \tag{3.26}$$

with $W_n(z)$ as defined in (3.17). Note that we have written the result for $E_{n,1}^{(j)}$ differently than for $E_{n,2}^{(j)}$ and $E_{n,3}^{(j)}$ since we cannot be sure that $W_n(c_{n+\mu+1}) \neq 0$. The asymptotic equalities for $E_{n,2}^{(j)}$ and $E_{n,3}^{(j)}$, however, are valid as $U_n(c_i) \neq 0$ for all $i \geq n+1$. The result now follows by substituting (3.26) in (3.23) and observing also that $E_{n,1}^{(j)} = o(E_{n,3}^{(j)})$ as $j \rightarrow \infty$, so that either $E_{n,2}^{(j)}$ or $E_{n,3}^{(j)}$ determines the asymptotic nature of $\dot{A}_n^{(j)} - \dot{A}$. We leave the details to the reader. \square

Remark. Comparing (3.19) pertaining to $\dot{A}_n^{(j)} - \dot{A}$ with (3.3) pertaining to $A_n^{(j)} - A$, we realize that, subject to the additional assumption in (3.12), the two behave practically the same way asymptotically. In addition, their computational costs are generally similar. (In many problems of interest $A(y)$

and $\dot{A}(y)$ can be computed simultaneously, the total cost of this being almost the same as that of computing $A(y)$ only or $\dot{A}(y)$ only. An immediate example is that of numerical integration discussed in Section 1.) In contrast, the convergence of $\{B_n^{(j)}\}_{j=0}^\infty$ obtained by applying GREP⁽²⁾ directly to $\dot{A}(y) \equiv \dot{a}(t)$ (recall (2.18) and (2.19)), is inferior to that of $\{A_n^{(j)}\}_{j=0}^\infty$. This can be shown rigorously for the case in which $\dot{\phi}(y) \equiv \dot{\phi}(t) = K\varphi(t)(\log t + \text{constant})$ exactly. In this case the asymptotic expansion in (2.18) assumes the form $\dot{a}(t) \sim \dot{A} + \sum_{k=1}^\infty \varphi(t)(\alpha_{k0} + \alpha_{k1} \log t)t^k$ as $t \rightarrow 0+$. Therefore, under the additional condition that $\lim_{m \rightarrow \infty} \varepsilon_m \log t_m = 0$, where ε_m is as defined following (3.12), Theorem 2.2 of [11] applies and we have

$$B_{2m}^{(j)} - B = O(\varphi(t_j)t_j^m \log t_j) \quad \text{as } j \rightarrow \infty. \tag{3.27}$$

Now the computational costs of $\dot{A}_{2m}^{(j)}$ and $B_{2m}^{(j)}$ are similar, but $\{\dot{A}_{2m}^{(j)}\}_{j=0}^\infty$ converges to \dot{A} much faster than $\{B_{2m}^{(j)}\}_{j=0}^\infty$. Again, we have verified the superiority of our new approach to the direct approach, at least with respect to column sequences.

We would like to add that the theory of [11] applies to the more general class of functions $A(y)$ that have asymptotic expansions of the form $A(y) \sim A + \sum_{k=1}^\infty \psi_k(y)(\sum_{i=0}^{q_k} \alpha_{ki}(\log y)^i)$ as $y \rightarrow 0+$, where q_k are arbitrary nonnegative integers.

4. Application to infinite series via the $d^{(1)}$ -transformation: the $(d/d\xi)d^{(1)}$ -transformation

4.1. General usage

Let $\{S_m\}$ be the sequence of partial sums of the infinite series $\sum_{k=1}^\infty v_k$, namely,

$$S_m = \sum_{k=1}^m v_k, \quad m = 1, 2, \dots \tag{4.1}$$

Assume that

$$v_m \sim \sum_{i=0}^\infty \theta_i m^{\rho-i} \quad \text{as } m \rightarrow \infty, \quad \theta_0 \neq 0, \quad \rho + 1 \neq 0, 1, 2, \dots \tag{4.2}$$

As is known, $\lim_{m \rightarrow \infty} S_m$ exists and is finite if and only if $\Re \rho + 1 < 0$. When $\Re \rho + 1 \geq 0$ but $\rho + 1 \neq 0, 1, 2, \dots$, $\{S_m\}$ diverges but has a well defined and useful antilimit as has been shown in Theorem 4.1 of [10]. For all ρ in (4.2) this theorem reads as follows:

Theorem 4.1. *With S_m as in (4.1) and (4.2), we have*

$$S_m \sim S + mv_m \sum_{i=0}^\infty \beta_i m^{-i} \quad \text{as } m \rightarrow \infty, \quad \beta_0 \neq 0. \tag{4.3}$$

Here $S = \lim_{m \rightarrow \infty} S_m$ when $\Re \rho + 1 < 0$, and S is the antilimit of $\{S_m\}$ otherwise.

The part of Theorem 4.1 concerning convergent sequences $\{S_m\}$ is already contained in Theorem 2 of [6].

From Theorem 4.1 it is clear that GREP⁽¹⁾ can be applied to the sequence $\{S_m\}$ by drawing the analogy $a(t) \leftrightarrow S_m$, $t \leftrightarrow m^{-1}$, $\varphi(t) \leftrightarrow mv_m$, and $A \leftrightarrow S$, and by picking $t_l = 1/R_l$ for some positive integers R_l , $1 \leq R_0 < R_1 < R_2 < \dots$, and the W -algorithm can be used to implement it. This GREP⁽¹⁾ is simply the Levin–Sidi $d^{(1)}$ -transformation, and we denote its $A_n^{(j)}$ by $S_n^{(j)}$.

As already explained in [10,4], for the type of sequences considered here we should pick the R_l such that $\{R_l\}$ increases exponentially to ensure the best stability and convergence properties in the $S_n^{(j)}$. Exponential increase in the R_l can be achieved by picking them, for example, as in

$$R_0 = 1 \quad \text{and} \quad R_{l+1} = \lfloor \sigma R_l \rfloor + 1, \quad l = 0, 1, \dots, \quad \text{for some } \sigma > 1. \tag{4.4}$$

(With $\sigma = 1$ we have $R_l = l + 1$, $l = 0, 1, \dots$, for which the $d^{(1)}$ -transformation becomes the Levin [5] u -transformation.) This gives $R_l = O(\sigma^l)$ as $l \rightarrow \infty$. Needless to say, σ should not be picked too far from 1 to avoid too quick a growth in the R_l . We have found that σ between 1.1 and 1.5 is sufficient for most purposes. Since $t_l = 1/R_l$, (4.4) implies that

$$\frac{t_l}{\sigma + t_l} \leq t_{l+1} < \frac{t_l}{\sigma}, \quad l = 0, 1, \dots \tag{4.5}$$

as a result of which $\{t_l\}$ satisfies (3.1) with $\omega = 1/\sigma \in (0, 1)$. Therefore, Theorem 3.1 applies to the approximations $S_m^{(j)}$ to S obtained via the $d^{(1)}$ -transformation, as has been shown in [10]. Clearly, $\delta = -\rho - 1$ in (3.2) and (3.6) for this case.

If, in addition, v_m and S are differentiable functions of a parameter ξ , \dot{S} is the limit or antilimit of $\{\dot{S}_m\}$, and

$$\dot{v}_m = v_m[K' \log m + L' + o(1)] \quad \text{as } m \rightarrow \infty, \quad \text{for some constants } K' \neq 0 \text{ and } L' \tag{4.6}$$

and the asymptotic expansion in (4.3) can be differentiated with respect to ξ term by term, then Theorems 3.2–3.4 apply to $\{\dot{S}_n^{(j)}\}_{j=0}^\infty$ without any modifications. We shall denote this method that produces the $\dot{S}_n^{(j)}$ the $(d/d\xi)d^{(1)}$ -transformation for short. The rate of convergence of the $\dot{S}_n^{(j)}$ to \dot{S} is almost identical to the rate of convergence of the $S_n^{(j)}$ to S as we have observed in many numerical examples, and as we have proved in Theorem 3.4 for the column sequences.

To summarize the relevant convergence results for the $d^{(1)}$ - and $(d/d\xi)d^{(1)}$ -transformations as these are applied to $\{S_m\}$ and $\{\dot{S}_m\}$ above, we have from Theorems 3.1 and 3.4

$$\begin{aligned} S_n^{(j)} - S &= O(v_{R_j} R_j^{-n+1}) = O(\sigma^{(\rho+1-n)j}) \quad \text{as } j \rightarrow \infty, \\ \dot{S}_n^{(j)} - \dot{S} &= O(v_{R_j} R_j^{-n+1} \log R_j) = O(j\sigma^{(\rho+1-n)j}) \quad \text{as } j \rightarrow \infty. \end{aligned} \tag{4.7}$$

Of course, these results are not optimal. Optimal results follow from (3.3) and (3.19), and we leave them to the reader. The results for $\Gamma_n^{(j)}$ and $\Omega_n^{(j)}$ that pertain to stability can be obtained from Theorems 3.1–3.3.

For the sake of completeness we note that the $(d/d\xi)W$ -algorithm takes $t_j = 1/R_j$, $a(t_j) = \sum_{k=1}^{R_j} v_k$, $\dot{a}(t_j) = \sum_{k=1}^{R_j} \dot{v}_k$, $\varphi(t_j) = R_j v_{R_j}$, and $\dot{\varphi}(t_j) = R_j \dot{v}_{R_j}$ as input for this problem.

It is worth mentioning that we can also compute \dot{S} by applying the $d^{(2)}$ -transformation directly to $\{\dot{S}_m\}$. The $d^{(2)}$ -transformation is a GREP⁽²⁾. As we mentioned earlier, this is less effective than the application of the $(d/d\xi)d^{(1)}$ -transformation to $\{S_m\}$. We shall see this also through numerical examples in the next section.

4.2. A special application

We next turn to an interesting application of the $(d/d\xi)d^{(1)}$ -transformation to the summation of a class of infinite series $\sum_{k=1}^{\infty} \tilde{v}_k$, where \tilde{v}_m has the form

$$\tilde{v}_m = [\log \mu(m)]v_m, \quad \mu(m) \sim \sum_{i=0}^{\infty} \mu_i m^{\alpha-i} \quad \text{as } m \rightarrow \infty, \quad \mu_0 \neq 0 \text{ and } \alpha \neq 0, \tag{4.8}$$

with v_m as in (4.2). (When $\alpha = 0$ the $d^{(1)}$ -transformation is very effective on the series $\sum_{k=1}^{\infty} \tilde{v}_k$.) To this end first let us consider the infinite series $\sum_{k=1}^{\infty} u_k(\xi)$, where

$$u_m(\xi) = v_m[\mu(m)]^{\xi}, \quad m = 1, 2, \dots \tag{4.9}$$

(Here v_m and $\mu(m)$ do not depend on ξ). Now it can be shown that $[\mu(m)]^{\xi} \sim \sum_{i=0}^{\infty} \mu'_i m^{\varepsilon-i}$ as $m \rightarrow \infty$, where $\mu'_0 = \mu_0^{\xi} \neq 0$ and $\varepsilon = \alpha\xi$. Consequently, $u_m(\xi) \sim \sum_{i=0}^{\infty} \theta'_i m^{\rho'-i}$ as $m \rightarrow \infty$, where $\theta'_0 = \theta_0 \mu_0^{\xi} \neq 0$ and $\rho' = \rho + \alpha\xi$, so that $u_m(\xi)$ is of the form described in (4.1) for all ξ . That is to say, the $d^{(1)}$ -transformation can be applied to sum $\sum_{k=1}^{\infty} u_k(\xi)$ for any ξ . Next, $\dot{u}_m(\xi) = u_m(\xi) \log \mu(m) \sim u_m(\xi)[\alpha \log m + \log \mu_0 + o(1)]$ as $m \rightarrow \infty$, cf. (4.6). Therefore, the $(d/d\xi)d^{(1)}$ -transformation can be used for summing $\sum_{k=1}^{\infty} \dot{u}_k(\xi)$ for any ξ . Finally, $u_m(0) = v_m$ and $\dot{u}_m(0) = \tilde{v}_m$, and hence the $(d/d\xi)d^{(1)}$ -transformation can be used for summing $\sum_{k=1}^{\infty} \tilde{v}_k$ in particular. This can be done by setting $t_j = 1/R_j$, $a(t_j) = \sum_{k=1}^{R_j} v_k$, $\dot{a}(t_j) = \sum_{k=1}^{R_j} \tilde{v}_k$, $\varphi(t_j) = R_j v_{R_j}$, and $\dot{\varphi}(t_j) = R_j \tilde{v}_{R_j}$ in the $(d/d\xi)W$ -algorithm.

5. Numerical examples

In this section we wish to demonstrate numerically the effectiveness of $(d/d\xi)GREP^{(1)}$ via the $(d/d\xi)d^{(1)}$ -transformation on some infinite series, convergent or divergent. We will do this with two examples. The first one of these examples has already been treated in [14] within the framework of the Richardson extrapolation process.

Example 5.1. Consider the series $\sum_{k=1}^{\infty} k^{-\xi-1}$ that converges for $\Re \xi > 0$ and defines the Riemann zeta function $\zeta(\xi + 1)$. As is known, $\zeta(z)$ can be continued analytically to the entire complex plane except $z = 1$, where it has a simple pole. As the term $v_m = m^{-\xi-1}$ is of the form described in the previous section, Theorem 4.1 applies to $S_m = \sum_{k=1}^m k^{-\xi-1}$ with $S = \zeta(\xi + 1)$ and $\delta = \xi$, whether $\lim_{m \rightarrow \infty} S_m$ exists or not. Furthermore, the asymptotic expansion of $\dot{S}_m = \sum_{k=1}^m (-\log k) k^{-\xi-1}$ can be obtained by term-by-term differentiation of the expansion in (4.3), as has already been mentioned in [14]. This implies that the $(d/d\xi)d^{(1)}$ -transformation can be applied to the computation of $\dot{S} = \zeta'(\xi + 1)$, and Theorems 3.2–3.4 are valid with $\delta = \xi$. In particular, (4.7) is valid with $\rho = -\xi - 1$ there.

We applied the $(d/d\xi)d^{(1)}$ -transformation to this problem to compute $\dot{S} = \zeta'(\xi + 1)$. We picked the integers R_l as in (4.4) with $\sigma = 1.2$ there. We considered the two cases (i) $\xi = 1$ and (ii) $\xi = -0.5$. Note that in case (i) both $\lim_{m \rightarrow \infty} S_m$ and $\lim_{m \rightarrow \infty} \dot{S}_m$ exist and are $S = \zeta(2)$ and $\dot{S} = \zeta'(2)$, respectively, while in case (ii) these limits do not exist and $S = \zeta(0.5)$ and $\dot{S} = \zeta'(0.5)$ are the corresponding antilimits. We also applied the $d^{(2)}$ -transformation directly to $\{S_m\}$ with the same R_l 's, the resulting approximations being denoted $B_n^{(j)}$, as in (2.19). The numerical results are shown in Tables 1–3.

Table 1

Numerical results on Process I for $\zeta(z)$ in Example 5.1, where $\zeta(z)$ is the Riemann zeta function, with $z=2$. The $d^{(1)}$ - and $(d/d\xi)d^{(1)}$ -transformations on $\{S_m\}$ and $\{\dot{S}_m\}$ and the $d^{(2)}$ -transformation on $\{\dot{S}_m\}$ are implemented with $\sigma=1.2$ in (4.4). Here $P_n^{(j)} = |S_n^{(j+1)} - S|/|S_n^{(j)} - S|$, $Q_n^{(j)} = |\dot{S}_n^{(j+1)} - \dot{S}|/|\dot{S}_n^{(j)} - \dot{S}|$, and $Z_n^{(j)} = |B_n^{(j+1)} - \dot{S}|/|B_n^{(j)} - \dot{S}|$, where $S_n^{(j)}$, $\dot{S}_n^{(j)}$, and $B_n^{(j)}$ are the approximations obtained from the $d^{(1)}$ -, $(d/d\xi)d^{(1)}$ -, and $d^{(2)}$ -transformations, respectively. All six columns are tending to $\sigma^{-7} = 0.279\dots$

j	$P_5^{(j)}$	$Q_5^{(j)}$	$Z_{10}^{(j)}$	$P_6^{(j)}$	$Q_6^{(j)}$	$Z_{12}^{(j)}$
0	1.53D - 01	1.62D - 01	3.18D - 01	1.09D - 03	2.25D - 02	3.08D - 02
2	1.94D - 01	2.09D - 01	2.01D - 01	3.23D - 01	3.19D - 01	1.06D - 01
4	1.97D - 01	2.10D - 01	1.58D - 01	2.30D - 01	2.41D - 01	1.58D - 02
6	2.33D - 01	2.46D - 01	2.02D - 01	2.44D - 01	2.56D - 01	4.27D - 01
8	2.45D - 01	2.57D - 01	4.95D - 01	2.51D - 01	2.63D - 01	2.93D - 01
10	2.50D - 01	2.61D - 01	3.56D - 01	2.56D - 01	2.66D - 01	2.65D - 01
12	2.65D - 01	2.75D - 01	3.22D - 01	2.66D - 01	2.75D - 01	2.58D - 01
14	2.67D - 01	2.76D - 01	3.07D - 01	2.68D - 01	2.77D - 01	2.60D - 01
16	2.70D - 01	2.79D - 01	3.03D - 01	2.71D - 01	2.79D - 01	2.69D - 01
18	2.70D - 01	2.79D - 01	2.99D - 01	2.71D - 01	2.79D - 01	2.78D - 01
20	2.74D - 01	2.82D - 01	2.97D - 01	2.74D - 01	2.82D - 01	2.85D - 01

Table 2

Numerical results on Process II for $\zeta(z)$ in Example 5.1, where $\zeta(z)$ is the Riemann zeta function, with $z=2$. The $d^{(1)}$ - and $(d/d\xi)d^{(1)}$ -transformations on $\{S_m\}$ and $\{\dot{S}_m\}$ and the $d^{(2)}$ -transformation on $\{\dot{S}_m\}$ are implemented with $\sigma=1.2$ in (4.4). Here $S_n^{(j)}$, $\dot{S}_n^{(j)}$, and $B_n^{(j)}$ are the approximations obtained from the $d^{(1)}$ -, $(d/d\xi)d^{(1)}$ -, and $d^{(2)}$ -transformations, respectively. (The infinite series converge.)

n	R_n	$ S_{R_n} - S $	$ S_n^{(0)} - S $	$ \dot{S}_{R_n} - \dot{S} $	$ \dot{S}_n^{(0)} - \dot{S} $	$ B_n^{(0)} - \dot{S} $
0	1	6.45D - 01	1.64D + 00	9.38D - 01	9.38D - 01	9.38D - 01
2	3	2.84D - 01	1.99D - 02	6.42D - 01	3.67D - 02	4.56D - 01
4	5	1.81D - 01	3.12D - 05	4.91D - 01	1.07D - 04	3.28D - 03
6	9	1.05D - 01	7.08D - 07	3.42D - 01	1.56D - 06	6.19D - 04
8	14	6.89D - 02	8.18D - 09	2.53D - 01	2.35D - 08	3.26D - 05
10	21	4.65D - 02	3.71D - 11	1.89D - 01	1.25D - 10	8.26D - 07
12	32	3.08D - 02	6.95D - 14	1.38D - 01	2.70D - 13	5.11D - 07
14	47	2.11D - 02	2.55D - 17	1.02D - 01	1.44D - 16	4.17D - 09
16	69	1.44D - 02	8.28D - 20	7.54D - 02	3.03D - 19	1.60D - 11
18	100	9.95D - 03	1.14D - 22	5.58D - 02	4.90D - 22	4.32D - 13
20	146	6.83D - 03	5.75D - 26	4.09D - 02	2.72D - 25	2.14D - 16
22	212	4.71D - 03	1.52D - 29	2.99D - 02	4.53D - 29	4.53D - 17
24	307	3.25D - 03	2.44D - 30	2.19D - 02	3.52D - 29	1.97D - 19

Table 1 shows the validity of the theory for Process I given in Sections 2–4 very clearly. The results of this table that have been computed with $\xi = 1$ can be understood as follows:

Table 3

Numerical results on Process II for $\zeta(z)$ in Example 5.1, where $\zeta(z)$ is the Riemann zeta function, with $z = 0.5$. The $d^{(1)}$ - and $(d/d\xi)d^{(1)}$ -transformations on $\{S_m\}$ and $\{\dot{S}_m\}$ and the $d^{(2)}$ -transformation on $\{\dot{S}_m\}$ are implemented with $\sigma = 1.2$ in (4.4). Here $S_n^{(j)}$, $\dot{S}_n^{(j)}$, and $B_n^{(j)}$ are the approximations obtained from the $d^{(1)}$ -, $(d/d\xi)d^{(1)}$ -, and $d^{(2)}$ -transformations, respectively. (The infinite series diverge.)

n	R_n	$ S_{R_n} - S $	$ S_n^{(0)} - S $	$ \dot{S}_{R_n} - \dot{S} $	$ \dot{S}_n^{(0)} - \dot{S} $	$ B_n^{(0)} - \dot{S} $
0	1	2.46D + 00	1.46D + 00	3.92D + 00	3.92D + 00	3.92D + 00
2	3	3.74D + 00	1.28D - 01	2.80D + 00	1.65D - 01	5.33D - 01
4	5	4.69D + 00	1.01D - 03	1.39D + 00	4.64D - 04	9.62D + 00
6	9	6.17D + 00	4.71D - 06	1.55D + 00	9.73D - 06	2.50D + 00
8	14	7.62D + 00	2.32D - 07	5.13D + 00	8.13D - 08	1.05D + 00
10	21	9.27D + 00	2.24D - 09	9.90D + 00	4.19D - 10	2.01D - 01
12	32	1.14D + 01	8.85D - 12	1.69D + 01	5.88D - 12	4.02D - 02
14	47	1.38D + 01	1.33D - 14	2.56D + 01	1.71D - 14	1.79D - 03
16	69	1.67D + 01	2.51D - 18	3.74D + 01	8.66D - 18	1.41D - 05
18	100	2.00D + 01	2.74D - 20	5.23D + 01	2.88D - 20	1.50D - 07
20	146	2.42D + 01	2.76D - 23	7.23D + 01	4.34D - 23	1.91D - 09
22	212	2.92D + 01	6.72D - 27	9.79D + 01	3.13D - 26	2.21D - 11
24	307	3.51D + 01	6.38D - 27	1.31D + 02	1.54D - 26	1.41D - 13

Since

$$S_{n-1} \sim \zeta(\xi + 1) - \frac{n^\xi}{\xi} \sum_{i=0}^{\infty} \binom{-\xi}{i} B_i n^{-i} \quad \text{as } n \rightarrow \infty,$$

and since $B_0 = 1$, $B_1 = -\frac{1}{2}$, while $B_{2i} \neq 0$, $B_{2i+1} = 0$, $i = 1, 2, \dots$, we have that with the exception of β_{2i+1} , $i = 1, 2, \dots$, all the other β_i are nonzero, and that exactly the same applies to the $\dot{\beta}_i$. (Here B_i are the Bernoulli numbers and should not be confused with $B_n^{(j)}$.) Consequently, (3.19) of Theorem 3.4 holds with $\mu = \nu$ there. Thus, whether $\lim_{m \rightarrow \infty} S_m$ exists or not, as $j \rightarrow \infty$, $|S_n^{(j+1)} - S|/|S_n^{(j)} - S|$ is $O(\sigma^{-1})$ for $n = 0$, $O(\sigma^{-2})$ for $n = 1$, $O(\sigma^{-3})$ for $n = 2$, and $O(\sigma^{-(2i+1)})$ for both $n = 2i - 1$ and $n = 2i$, with $i = 2, 3, \dots$. Similarly, whether $\lim_{m \rightarrow \infty} \dot{S}_m$ exists or not, as $j \rightarrow \infty$, $|\dot{S}_n^{(j+1)} - \dot{S}|/|\dot{S}_n^{(j)} - \dot{S}|$ is $O(\sigma^{-1})$ for $n = 0$, $O(\sigma^{-2})$ for $n = 1$, $O(\sigma^{-3})$ for $n = 2$, and $O(\sigma^{-(2i+1)})$ for both $n = 2i - 1$ and $2i$, with $i = 2, 3, \dots$.

As for the approximations $B_n^{(j)}$ to \dot{S} obtained from the $d^{(2)}$ -transformation on $\{\dot{S}_m\}$, Theorem 2.2 in [11] implies that, as $j \rightarrow \infty$, $|B_n^{(j+1)} - \dot{S}|/|B_n^{(j)} - \dot{S}|$ is $O(\sigma^{-1})$ for $n = 0$, $O(\sigma^{-2})$ for $n = 2$, $O(\sigma^{-3})$ for $n = 4$, and $O(\sigma^{-(2i+1)})$ for both $n = 2(2i - 1)$ and $n = 4i$, with $i = 2, 3, \dots$.

The numerical results of Tables 2 and 3 pertain to Process II and show clearly that our approach to the computation of derivatives of limits is a very effective one.

Example 5.2. Consider the summation of the infinite series $\sum_{k=0}^{\infty} \dot{v}_k$, where $v_m = b_m(\xi)_m/m!$ and $(\xi)_m = \prod_{i=0}^{m-1} (\xi + i)$, and $b_m \sim \sum_{i=0}^{\infty} \kappa_i m^{\eta-i}$ as $m \rightarrow \infty$. By the fact that $(\xi)_m = \Gamma(\xi + m)/\Gamma(\xi)$ and by formula 6.1.47 in [1] we have that $(\xi)_m/m! \sim \sum_{i=0}^{\infty} \lambda_i m^{\xi-i-1}$ as $m \rightarrow \infty$. Consequently, $v_m \sim \sum_{i=0}^{\infty} \theta_i m^{\eta+\xi-1-i}$ as $m \rightarrow \infty$, so that the $d^{(1)}$ -transformation can be applied successfully to sum

Table 4

Numerical results on Process II for $F(\xi, \frac{1}{2}; \frac{3}{2}; 1)$ in Example 5.2, where $F(a, b; c; z)$ is the Gauss hypergeometric function, with $\xi = 0.5$. The $d^{(1)}$ - and $(d/d\xi)d^{(1)}$ -transformations on $\{S_m\}$ and $\{\dot{S}_m\}$ and the $d^{(2)}$ -transformation on $\{S_m\}$ are implemented with $\sigma = 1.2$ in (4.4). Here $S_n^{(j)}$, $\dot{S}_n^{(j)}$, and $B_n^{(j)}$ are the approximations obtained from the $d^{(1)}$ -, $(d/d\xi)d^{(1)}$ -, and $d^{(2)}$ -transformations, respectively. (The infinite series converge.)

n	R_n	$ S_{R_n} - S $	$ S_n^{(0)} - S $	$ \dot{S}_{R_n} - \dot{S} $	$ \dot{S}_n^{(0)} - \dot{S} $	$ B_n^{(0)} - \dot{S} $
0	1	5.71D - 01	1.57D + 00	2.18D + 00	2.18D + 00	2.18D + 00
2	3	3.29D - 01	4.70D - 02	1.64D + 00	2.18D - 01	6.79D - 01
4	5	2.54D - 01	4.06D - 05	1.41D + 00	4.06D - 04	1.51D - 01
6	9	1.89D - 01	1.69D - 06	1.16D + 00	1.22D - 05	4.59D - 02
8	14	1.51D - 01	1.95D - 08	9.96D - 01	1.39D - 07	3.76D - 03
10	21	1.23D - 01	1.11D - 10	8.63D - 01	7.94D - 10	1.47D - 04
12	32	9.99D - 02	3.11D - 13	7.41D - 01	2.20D - 12	4.42D - 06
14	47	8.24D - 02	3.99D - 16	6.43D - 01	2.61D - 15	9.14D - 08
16	69	6.80D - 02	1.20D - 19	5.57D - 01	1.41D - 19	1.26D - 09
18	100	5.64D - 02	2.04D - 22	4.84D - 01	2.38D - 21	1.57D - 11
20	146	4.67D - 02	2.03D - 25	4.18D - 01	2.03D - 24	2.21D - 13
22	212	3.88D - 02	6.77D - 29	3.61D - 01	7.81D - 28	1.86D - 15
24	307	3.22D - 02	2.41D - 29	3.12D - 01	1.51D - 28	1.13D - 18

$\sum_{k=0}^{\infty} v_k$, as described in the previous section. Now $\dot{v}_m = v_m[\sum_{i=0}^{m-1} 1/(\xi + i)]$, and $\sum_{i=0}^{m-1} 1/(\xi + i) \sim \log m + \sum_{k=0}^{\infty} e_k m^{-k}$ as $m \rightarrow \infty$. Therefore, we can apply the $(d/d\xi)d^{(1)}$ -transformation to sum $\sum_{k=0}^{\infty} \dot{v}_k$ provided that the asymptotic expansion of \dot{S}_m can be obtained by term-by-term differentiation by Theorem 4.1. (We have not shown that this last condition is satisfied).

We have applied the $(d/d\xi)d^{(1)}$ -transformation with $b_m = 1/(2m + 1)$. With this b_m the series $\sum_{k=0}^{\infty} v_k$ and $\sum_{k=0}^{\infty} \dot{v}_k$ both converge. Actually we have $\sum_{k=0}^{\infty} v_k = F(\xi, \frac{1}{2}; \frac{3}{2}; 1)$. By formula 15.1.20 in [1], $\sum_{k=0}^{\infty} v_k = (\sqrt{\pi}/2)(\Gamma(1 - \xi)/\Gamma(3/2 - \xi)) = S$. Differentiating both sides with respect to ξ , we obtain $\sum_{k=0}^{\infty} \dot{v}_k = (\sqrt{\pi}/2)(\Gamma(1 - \xi)/\Gamma(3/2 - \xi))\{\psi(\frac{3}{2} - \xi) - \psi(1 - \xi)\} = \dot{S}$, where $\psi(z) = (d/dz)\Gamma(z)/\Gamma(z)$. Letting now $\xi = \frac{1}{2}$ throughout, we get $S = \pi/2$ and $\dot{S} = \pi \log 2$, the latter following from formulas 6.3.2 and 6.3.3 in [1].

In our computations we picked the R_l as in the first example. We also applied the $d^{(2)}$ -transformation directly to $\{\dot{S}_m\}$ with the same R_l 's.

Table 4 contains numerical results pertaining to Process II.

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Matrix Hermite–Padé problem and dynamical systems

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Abstract

The solution of a discrete dynamical system is studied. To do so spectral properties of the band operator, with intermediate zero diagonals, are investigated. The method of genetic sums for the moments of the Weyl function is used to find the continued fraction associated to this Weyl function. It is possible to follow the inverse spectral method to solve dynamical systems defined by a Lax pair. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Let us consider the infinite system (E) of differential equations, for $n = 0, 1, \dots$,

$$(E) \quad \begin{aligned} b'_{n+3} &= b_{n+3}(U_{n+3} - U_{n-2}), \\ U_{n+3} &= b_{n+6}(b_{n+9} + b_{n+7} + b_{n+5}) + b_{n+4}(b_{n+7} + b_{n+5}) + b_{n+2}b_{n+5}, \end{aligned}$$

where the solutions $b_{n+3}(t)$ are unknown real functions of t , $t \in [0, +\infty[$ with conditions $b_{n+3}(t) = 0$, $n < 0$. These conditions are boundary conditions with respect to n for system (E). We formulate the Cauchy problem for system (E), i.e., with initial conditions

$$b_{n+3}(0), \quad n \geq 0.$$

Why are we interested in such dynamical system? Bogoyavlensky [4,5] has given a classification of all dynamical systems which are a discrete generalization of the KdV equation; they depend on two parameters p and q . He showed that such systems have interesting applications in hamiltonian mechanics.

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Our system is such a dynamical system for $p = 3, q = 2$. This case includes the main ideas of the general case. In Section 7, we give different transformations of system (E). For $p = q = 1$, we get the Langmuir chain [9], for $p = 1$ and q any integer or $q = 1$ and p any integer, the systems have been studied, respectively, by Sorokin [11] and by Aptekarev [1]:

$$p = 1, \quad a'_n = a_n \left(\prod_{k=1}^q a_{n+k} - \prod_{k=1}^q a_{n-k} \right),$$

$$q = 1, \quad a'_n = a_n \left(\sum_{k=1}^p a_{n+k} - \sum_{k=1}^p a_{n-k} \right).$$

In order to be explicit, we will often restrict to the case $p = 3, q = 2$, the important assumption being that p and q are relatively prime. Studies of the same kind, with no references to dynamical systems, but concerned with the finite-dimensional approximations of the resolvent of an infinite three diagonal band matrix can be found in [3, 2]. What we call in our notation the matrix $A(3)$ has three diagonals (i.e., $p = q = 1$), but nonbounded or even complex data are considered. We have not considered nonbounded operators in this paper.

The first natural question for a Cauchy problem is the existence and uniqueness of the solution. A classical theory of ODE does not give the answer because system (E) is infinite.

We will prove two results through this paper.

Theorem A. *If all $b_{n+3}(0)$ are positive, bounded*

$$0 < b_{n+3}(0) \leq M, \quad n \geq 0,$$

then the Cauchy problem for system (E) has a unique solution defined on $[0, +\infty[$.

As usual, it is possible to prove only the local existence and uniqueness of the solution of discrete dynamical systems [8]. As a remark, in the case where all $b_{n+3}(0)$ are not positive, there exists examples where the solution is not unique, so the condition is not only sufficient but also necessary. In physical applications, the b_{n+3} are exponents of physical data, so are positive.

If the $(b_{n+3}(0))_{n \geq 0}$ are not bounded, then the solution does not extend beyond some interval $[0, t_1]$. In this paper, we do not consider this case, which would be possible following the same scheme, but the theory of operators, in case of an unbounded, nonsymmetric operator, is to be used, and yet there do not exist sufficient results.

The next question is how to find the solution of system (E). Tools are known, it is the inverse spectral problem. In this paper, we give the solution in classical form, in terms of continued fraction, as for the Langmuir chain. We get (the matrix Φ of constants will be defined in the text (7) and the notation F/z^Φ means that each component is $f^{i,j}/z^{\Phi^{i,j}}$)

Theorem B. *The solution of system (E) is*

$$F(z) = \frac{1}{z^\Phi} \int \frac{d\mu(x, t)}{z - x} = \frac{I_3}{P+} \frac{C_1}{P+} \frac{C_2}{P + \dots}, \tag{1}$$

where

$$d\mu(x, t) = \frac{e^{x^5 t} d\mu(x)}{\int e^{x^5 t} d\mu^{1,1}(x)}, \quad P = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & z \end{pmatrix}, \quad C_n = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -b_{n+2} \end{pmatrix}$$

and $d\mu$ is a matrix $(p \times q) = (3 \times 2)$ of positive measures.

What is a matrix continued fraction is explained in Section 5 [6,13,15]. So Theorem B means that from the initial conditions $b_{n+3}(0)$, we compute the continued fraction (i.e., solve the direct spectral problem), then write the result as the Cauchy transform of the matrix measure. Then using simple dynamics of this measure, we decompose the Cauchy integral into a continued fraction (solve the inverse spectral problem) and get $b_{n+3}(t)$ for $t \in [0, +\infty[$.

Theorem B has two aspects, the first is algebraic, namely the algorithm of construction of the matrix continued fraction, the second is analytic, i.e., we get a positive measure. This aspect deals with zeros properties of the convergents of the continued fraction (see Section 6), which are Hermite–Padé approximants [10,12], of the function F on the left-hand side of (1). So, we begin our paper by the definition of these approximants in Sections 2 and 3.

Theorems A and B are in fact proved simultaneously. In Theorem B we have the solution of system (E) on $[0, +\infty[$ but not the uniqueness. A local theorem gives existence and uniqueness on some segment $[0, t_0]$, and its length depends only on the constant M . If $b_{n+3}(t_0)$ are known to be positive bounded by the same constant M , then $b_{n+3}(t)$ can be extended on the segment $[t_0, 2t_0]$ and so on. Such information is obtained from Theorem B, using techniques of genetic sums (Section 4) [14]. So in complement of the preceding results, we also have

$$0 < b_{n+3}(t) \leq M, \quad t \in [0, +\infty[, \quad n \geq 0.$$

To get the dynamics of the spectral measure $d\mu$ in (1), we need the following differential equation satisfied by its power moments, $S_n = \int x^{5n} d\mu(x, t) = (S_n^{i,j})$, $i = 1, 2, 3$; $j = 1, 2$ the matrices being

$$S'_n = S_{n+1} - S_n S_1^{1,1}, \quad n = 0, 1, \dots \tag{2}$$

How to prove that systems (E) and (2) are equivalent? We use the standard method of Lax pairs. We consider the bi-infinite matrix

$$A = \begin{pmatrix} 0 & 0 & 0 & a_0 & \cdots & & & & \\ & \cdots & \cdots & \cdots & \ddots & & & & \\ b_p & 0 & & & & a_p & \cdots & & \\ & \ddots & & & & & \ddots & & \end{pmatrix}, \tag{3}$$

where for system (E) $a_n = 1$ (but it is possible to consider another normalization), and look for an infinite matrix B such that system (E) can be rewritten in the form

$$A' = [A, B],$$

where $[A, B] = AB - BA$. There exists such matrix B for our system and it is constructed in Section 7. Then we have

$$(A^n)' = [A^n, B]$$

which is proved by recurrence. Then the resolvent operator can be expanded in a neighbourhood of infinity,

$$R_z = (zI - A)^{-1} = \sum_{n=0}^{\infty} \frac{A^n}{z^{n+1}},$$

hence

$$R'_z = [R_z, B]. \tag{4}$$

But the function F on the left-hand side of (1) is the top left corner of R_z (as $f^{i,j} = (R_z e_{i-1}, e_{j-1})$) and (4), in particular, means, with Φ defined in (7)

$$F' = z^5 \left(F - \frac{S_0}{z^{\phi+1}} \right) - S_1^{1,1} F,$$

which is equivalent to (2).

We see that the solution of system (E) is found through the theory of Hermite–Padé approximants for which new results are proved: genetic sums, zeros properties.

2. The matrix Hermite–Padé problem

We define a matrix of power series with complex coefficients

$$F = \begin{pmatrix} f^{1,1} & \dots & f^{1,q} \\ \dots & \dots & \dots \\ f^{p,1} & \dots & f^{p,q} \end{pmatrix}, \quad f^{i,j}(z) = \sum_{n=0}^{\infty} \frac{f_n^{i,j}}{z^{n+1}}.$$

In matrix form

$$F = \sum_{n=0}^{\infty} \frac{f_n}{z^{n+1}}, \quad f_n = (f_n^{i,j})_{i=1, \dots, p; j=1, \dots, q}.$$

We now consider the Hermite–Padé problem (H–P) for F : for any $n \geq 0$, two regular multiindices are defined, i.e., $\vec{N} = (n_1, \dots, n_p)$ and $\vec{M} = (m_1, \dots, m_q)$ such that

$$\sum_1^p n_i = n, \quad n_1 \geq n_2 \geq \dots \geq n_p \geq n_1 - 1,$$

$$\sum_1^q m_i = n + 1, \quad m_1 \geq m_2 \geq \dots \geq m_q \geq m_1 - 1$$

(the Hermite–Padé problem can be considered for any indices, but we will restrict the study to the case of regular multiindices). We look for polynomials H_n^1, \dots, H_n^q not equal zero simultaneously, of degree not greater than $m_1 - 1, \dots, m_q - 1$, such that for some polynomials K_n^1, \dots, K_n^p the following

conditions hold:

$$\begin{aligned}
 R_n^1 &= f^{1,1}H_n^1 + \dots + f^{1,q}H_n^q - K_n^1 = O(1/z^{n_1+1}), \\
 &\vdots \\
 R_n^p &= f^{p,1}H_n^1 + \dots + f^{p,q}H_n^q - K_n^p = O(1/z^{n_p+1}).
 \end{aligned}$$

There always exists a nontrivial solution to this problem.

Considering the vectors $R_n = (R_n^1, \dots, R_n^p)^t$, $K_n = (K_n^1, \dots, K_n^p)^t$ and $H_n = (H_n^1, \dots, H_n^q)^t$, we get with matrix notation

$$R_n = FH_n - K_n = O(1/z^{\bar{N}+1}),$$

$$\deg H_n \leq \bar{M} - 1.$$

We consider $\mathbf{C}[X]^q$ the sets of column vectors of size q and their canonical basis

$$h_0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad h_1 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \dots, \quad h_{q-1} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}, \quad h_q = \begin{pmatrix} x \\ 0 \\ \vdots \\ 0 \end{pmatrix} \dots,$$

i.e., if $n = rq + s$, $s < q$, the components of h_n are zero except the component of index s which is equal to x^r , the components being numbered from 0 to $q - 1$. The same thing is done for $\mathbf{C}[X]^p$ and its canonical basis is denoted by e_n , $n \geq 0$, column vectors of size p .

The matrix moments f_n define the generalized Hankel \mathcal{H} matrix in block form and in scalar form, and for any n positive \mathcal{H}_n is the $n \times n$ minor in the upper left-hand corner

$$\mathcal{H} = \begin{pmatrix} f_0 & f_1 & f_2 & \dots \\ f_1 & f_2 & f_3 & \dots \\ \vdots & \vdots & \vdots & \dots \end{pmatrix} = \begin{pmatrix} h^{0,0} & h^{0,1} & h^{0,2} & \dots \\ h^{1,0} & h^{1,1} & h^{1,2} & \dots \\ \vdots & \vdots & \vdots & \dots \end{pmatrix} \tag{5}$$

and we define the bilinear functional

$$\Theta : \mathbf{C}[X]^p \times \mathbf{C}[X]^q \rightarrow \mathbf{C}, \quad \Theta(e_l, h_k) = \langle e_l, h_k \rangle_\Theta = h^{l,k},$$

where $l, k \geq 0$.

The H–P problem is equivalent to the orthogonality relations

$$H_n \in \text{Span}(h_0, \dots, h_n), \quad \Theta(e_k, H_n) = 0, \quad k = 0, \dots, n - 1. \tag{6}$$

We will restrict the study to the “ $(p|q)$ symmetric” case, i.e., the functions $f^{i,j}$ are, up to a shift, functions of z^{p+q} . Let a system S of $p \times q$ real sequences $(S_n^{i,j})_n$ be given for $i = 1, \dots, p$; $j = 1, \dots, q$. The parameters p and q are supposed to be relatively prime, so there exist integers u and v such

that

$$up - vq = 1.$$

According to what is found for the Weyl function F , we define the constants

$$\Phi^{i,j} = (j - i)(u + v) \bmod (p + q), \quad i = 1, \dots, p; \quad j = 1, \dots, q \tag{7}$$

and the $f^{i,j}$ are

$$f^{i,j}(z) = \sum_{n=0}^{\infty} \frac{S_n^{i,j}}{z^{(p+q)n + \Phi^{i,j} + 1}}.$$

Example 2.1. In the scalar case $p = q = 1$, $f^{1,1}$ is a symmetric function $f^{1,1}(z) = \sum_{n=0}^{\infty} S_n^{1,1} / z^{2n+1}$.

Example 2.2. In the vector case $p = 2, q = 1$,

$$f^{1,1}(z) = \sum_{n=0}^{\infty} \frac{S_n^{1,1}}{z^{3n+1}}, \quad f^{2,1}(z) = \sum_{n=0}^{\infty} \frac{S_n^{2,1}}{z^{3n+2}}.$$

Example 2.3. In the matrix case $p = 3, q = 2$, we get

$$f^{1,1}(z) = \sum_{n=0}^{\infty} \frac{S_n^{1,1}}{z^{5n+1}}, \quad f^{1,2}(z) = \sum_{n=0}^{\infty} \frac{S_n^{1,2}}{z^{5n+3}},$$

$$f^{2,1}(z) = \sum_{n=0}^{\infty} \frac{S_n^{2,1}}{z^{5n+4}}, \quad f^{2,2}(z) = \sum_{n=0}^{\infty} \frac{S_n^{2,2}}{z^{5n+1}},$$

$$f^{3,1}(z) = \sum_{n=0}^{\infty} \frac{S_n^{3,1}}{z^{5n+2}}, \quad f^{3,2}(z) = \sum_{n=0}^{\infty} \frac{S_n^{3,2}}{z^{5n+4}}.$$

As defined in (5), \mathcal{H}_n are the main $n \times n$ minors of \mathcal{H} , and we get the classical definition.

Definition 2.4. System S is called nonsingular or positive if, respectively,

$$\mathcal{H}_n \neq 0, \quad \mathcal{H}_n > 0.$$

Lemma 2.5. If S is nonsingular then

- The $(H-P)$ problem has a unique solution H_n (up to normalization).
- $\deg H_n = n$ with respect to the basis h_k .
- H_n is \mathbb{Z}_{p+q} -invariant, i.e., $H_n \in \text{Span}\{h_k, k = n \bmod (p + q)\}$.

The proof is a consequence of Cramer’s rule.

3. Generalized Jacobi matrix

We suppose the system S is nonsingular, and we get [12]

$$H_n = \frac{u_n}{\mathcal{H}_n} \begin{vmatrix} h^{0,0} & h^{0,1} & \dots & h^{0,n} \\ h^{1,0} & h^{1,1} & \dots & h^{1,n} \\ \vdots & \vdots & \vdots & \vdots \\ h^{n-1,0} & h^{n-1,1} & \dots & h^{n-1,n} \\ h_0 & h_1 & \dots & h_n \end{vmatrix}, \tag{8}$$

where the last row of the determinant is composed of vectors. The nonzero constants u_n are the leading coefficients of H_n (and may be changed in order to normalize the vector polynomials in one way or the other)

$$H_n = u_n h_n + \dots.$$

In [12] we have already got the following.

Theorem 3.1. *There exists a unique set of complex coefficients $a_n^{(m)}$, $m = -p, \dots, q$, $n \geq 0$, $n + m \geq 0$ such that the sequence of vector polynomials $(H_k)_k$ is the unique solution of the recurrence relation*

$$a_n^{(q)} H_{n+q} + \dots + a_n^{(1)} H_{n+1} + a_n^{(0)} H_n + a_n^{(-1)} H_{n-1} + \dots + a_n^{(-p)} H_{n-p} = x H_n \tag{9}$$

with the initial conditions

$$H_{-p} = \dots = H_{-1} = 0,$$

$$H_j = \frac{u_j}{\mathcal{H}_j} \begin{vmatrix} h^{0,0} & \dots & h^{0,j} \\ \vdots & \vdots & \vdots \\ h^{j-1,0} & \dots & h^{j-1,j} \\ h_0 & \dots & h_j \end{vmatrix}, \quad j = 0, \dots, q - 1.$$

In particular,

$$a_n^{(q)} = \frac{u_n}{u_{n+q}}, \quad n \geq 0,$$

$$a_{n+p}^{(-p)} = \frac{u_{n+p}}{u_n} \frac{\mathcal{H}_{n+p+1}}{\mathcal{H}_{n+p}} \frac{\mathcal{H}_n}{\mathcal{H}_{n+1}}, \quad n \geq 0. \tag{10}$$

Because here, only the symmetric case is considered, the result is simplified.

Theorem 3.2. *The sequence H_n is the unique solution of the recurrence relation*

$$x H_n = a_n H_{n+q} + b_n H_{n-p}, \tag{11}$$

with initial conditions

$$H_{-p} = \dots = H_{-1} = 0, \quad H_j = u_j h_j, \quad j = 0, \dots, q - 1.$$

a_n and b_n being defined as the $a_n^{(q)}, a_n^{(-p)}$ of the previous theorem.

The proof consists of the fact that $H = xH_n - bH_{n-p}$ satisfies the same orthogonality relations as H_{n+q} if $\langle e_{n-p}, H \rangle_\theta = 0$ (which defines b). It is also a consequence of the fact that xH_n, H_{n+q}, H_{n-p} are the only polynomials of (9) that depend on $h_k, k = n \bmod (p + q)$.

The recurrence relation (9) can be written in matrix form as

$$AH = xH, \tag{12}$$

where H is the infinite column vector $(H_0, H_1, \dots)^t$ (each term being a vector, H could be written as a scalar matrix $(\infty \times q)$) and A a scalar infinite band matrix with two nonzero diagonals,

$$A = \begin{pmatrix} 0 & \cdots & \cdots & a_0 & 0 & 0 \\ \vdots & 0 & \cdots & \cdots & a_1 & 0 \\ \vdots & & \ddots & & & \ddots \\ b_p & \cdots & \cdots & & & \\ 0 & b_{p+1} & \cdots & \cdots & & \\ 0 & 0 & \ddots & & & \end{pmatrix}.$$

From the relations in the previous theorem, a_n and b_n are positive if and only if the system S is positive (the vector polynomials H_n being considered with a positive normalization constant u_n). If, for the polynomials H_n , we take the monic polynomials ($u_n = 1$), then matrix A satisfies $a_n = 1$.

Another normalization will be used. If the leading coefficients of H_n are u_n , defined by

$$u_n = \left(\frac{\mathcal{H}_n}{\mathcal{H}_{n+1}} \right)^{p/(p+q)}$$

then [13]

$$(a_n \cdots a_{n+p-1})^q = (b_{n+p} \cdots b_{n+p+q-1})^p. \tag{13}$$

Such a matrix (two diagonals satisfying (13), $a_n > 0, b_n > 0$) generalizes the symmetric case and is called a generalized Jacobi matrix. If \mathcal{J} is the set of such matrices, and \mathcal{S} the set of the positive systems S normalized by $S_0^{1,1} = 1$, we have constructed a one-to-one correspondence (by the generalized Shohat–Favard theorem [12]) from \mathcal{S} to \mathcal{J} . In this case we will use the following representation of the parameters a_n and b_n , H_n^0 denoting the monic polynomials:

$$m_n = \langle e_n, H_n^0 \rangle, \quad u_n = (1/m_n)^{p/(p+q)},$$

$$c_n = \frac{m_{n+1}}{m_n}, \quad a_n = \left(\frac{m_{n+q}}{m_n} \right)^{p/(p+q)} = (c_n \cdots c_{n+q-1})^{p/(p+q)} = (\alpha_n)^{p/(p+q)},$$

$$b_{n+p} = \left(\frac{m_{n+p}}{m_n} \right)^{q/(p+q)} = (c_n \cdots c_{n+p-1})^{q/(p+q)} = (\beta_{n+p})^{q/(p+q)}.$$

The parameters c_n are uniquely defined if p and q are relatively prime.

4. Genetic sums

The aim of this section and the following is to give a representation by a matrix continued fraction, generalizing the S -fraction of Stieltjes, of the resolvent function of the operator defined in the standard basis of the Hilbert space $l_2(0, \infty)$ by the bi-infinite, $(p + q + 1)$ -band matrix A with $p + q - 1$ zero intermediate diagonals. The detailed proofs can be found in [14]. The matrix A is taken with the normalization giving $a_n = 1$, i.e., the matrix is defined by $A_{i,i+q} = 1$, $A_{i+p,i} = b_i$; equivalently the operator is defined by

$$A(e_i) = b_{i+p}e_{i+p}, \quad i < q, \quad A(e_i) = e_{i-q} + b_{i+p}e_{i+p}, \quad i \geq q,$$

where the constants b_i are a sequence of nonzero complex numbers. We assume that

$$\sup(|b_i|) < +\infty$$

to deal with bounded operators, and that p and q are relatively prime ($up - vq = 1$).

Let $R(z)$ be the resolvent operator,

$$R_z = (zI - A)^{-1}.$$

It is known [7] that the set of resolvent functions, the so-called Weyl functions

$$F = (f^{i,j}), \quad f^{i,j}(z) = \langle R_z e_{i-1}, e_{j-1} \rangle, \quad i = 1, \dots, p, \quad j = 1, \dots, q$$

can be chosen as spectral data, sufficient for the determination of the operator A given by the previous $(p + q + 1)$ -band matrix. The functions $f^{i,j}$ are analytic in the neighbourhood of infinity, because of the boundedness of A , and have power series expansions

$$f^{i,j}(z) = \sum_{n=0}^{\infty} \frac{f_n^{i,j}}{z^{n+1}}, \quad i = 1, \dots, p; \quad j = 1, \dots, q.$$

Hence, the formal solution of direct and inverse spectral problems means to find a constructive procedure for the determination of the spectral data $f^{i,j}$ or $f_n^{i,j}$ $i = 1, \dots, p; j = 1, \dots, q$ and $n \geq 0$ from the operator data b_n ($n \geq p$) and vice versa.

In the following, in order to give explicitly all the formulae, we will write everything for $p = 3$ and $q = 2$, but the results are general.

Because all the intermediate diagonals are zero, we are able to find a particular form for the moments called genetic sums [15]. This form has already been found for the vector case, recovered with $q = 1$ [1].

With the preceding notations, the moments, i.e., the coefficients $f_n^{i,j}$ of each function can be computed in terms of the b_i . Because the functions are found to be functions of the variable z^{p+q} , for each function $f^{i,j}$, all the coefficients, except a subsequence with indices $n(i, j)$, are zero. The results are as follows for $p = 3, q = 2$.

Theorem 4.1. *The moments of the Weyl functions associated to the operator A are given by the following: for all $n \geq 0$,*

$$n(1, 1) = 5n, \quad S_n^{1,1} = f_{n(1,1)}^{1,1} = b_3 \sum_{i_2} b_{i_2} \cdots \sum_{i_{2n}} b_{i_{2n}},$$

$$n(1, 2) = 2 + 5n, \quad S_n^{1,2} = f_{n(1,2)}^{1,2} = b_3 \sum_{i_1} b_{i_1} \cdots \sum_{i_{2n}} b_{i_{2n}},$$

$$n(2, 1) = 3 + 5n, \quad S_n^{2,1} = f_{n(2,1)}^{2,1} = b_4 \sum_{i_1} b_{i_1} \cdots \sum_{i_{2n}} b_{i_{2n}},$$

$$n(2, 2) = 5n, \quad S_n^{2,2} = f_{n(2,2)}^{2,2} = b_4 \sum_{i_2} b_{i_2} \cdots \sum_{i_{2n}} b_{i_{2n}},$$

$$n(3, 1) = 1 + 5n, \quad S_n^{3,1} = f_{n(3,1)}^{3,1} = \sum_{i_1} b_{i_1} \cdots \sum_{i_{3n}} b_{i_{3n}}, \quad i_1 \in \{3, 6\},$$

$$n(3, 2) = 3 + 5n, \quad S_n^{3,2} = f_{n(3,2)}^{3,2} = \sum_i b_i \sum_{i_1} b_{i_1} \cdots \sum_{i_{2n}} b_{i_{2n}}, \quad i \in \{3, 6\}$$

in all cases $i_k = i_{k-1} + p - \alpha q$, α integer, varying such that $1 \leq i_k \leq i_{k-1} + p$. In all other cases $f_k^{i,j} = 0$.

This means that $f^{i,j}$ are recovered as

$$f^{i,j}(z) = z^{p+q-\Phi^{i,j}-1} \sum_{n=0}^{\infty} \frac{S_n^{i,j}}{(z^{p+q})^{(n+1)}}.$$

The proof of these formulae can be found in [14]. The same method of proof leads to some identities for the genetic sums.

To the sequence $(b_n)_{n \geq p}$ is associated, for each pair (i, j) , $i = 1, \dots, p; j = 1, \dots, q$ the sequence $S_n^{i,j}$, $n \geq 0$, and similarly $S_n^{i,j}(k)$, $k \geq 0, n \geq 0$ corresponding to the sequence $(b_{n+k})_{n \geq p}$. Each family can be considered as the coefficients of a formal series and represented by this series, which defines $S^{i,j}(k)$ and $f^{i,j}(k)$:

$$S^{i,j}(k)(z) = \sum_{n \geq 0} \frac{S_n^{i,j}(k)}{z^{n+1}}, \quad i = 1, \dots, p; \quad j = 1, \dots, q, \quad k \geq 0. \tag{14}$$

What we are looking for is a relation between the matrix $F = (f^{i,j})_{i,j}$ and $F(1) = (f^{i,j}(1))_{i,j}$. We first obtain some relations between the moments $S_n^{i,j}$ and $S_n^{i,j}(1)$.

Lemma 4.2. *The following identities hold:*

$$S_{n+1}^{1,1} = b_3 \sum_{h=0}^n S_h^{1,1} S_{n-h}^{3,2}(1), \quad S_n^{1,2} = b_3 \sum_{h=0}^n S_h^{1,1} S_{n-h}^{3,1}(1),$$

$$S_n^{2,1} = \sum_{h=0}^n S_h^{2,1}(1) S_{n-h}^{1,1} k, \quad S_{n+1}^{2,2} = b_3 \sum_{h=0}^n S_h^{2,1} S_{n-h}^{3,1}(1) + S_{n+1}^{1,1}(1),$$

$$S_n^{3,1} = \sum_{h=0}^n S_h^{2,2}(1) S_{n-h}^{1,1}, \quad S_n^{3,2} = b_3 \sum_{h=0}^n S_h^{3,1} S_{n-h}^{3,1}(1) + S_n^{2,1}(1).$$

From these identities, some can be deduced for the functions $S^{i,j}(z)$ (and for the resolvent functions $f^{i,j}$).

Lemma 4.3. *The functions $S^{i,j}$ satisfy the identities*

$$S^{1,1} - \frac{1}{z} = b_3 S^{1,1} S^{3,2}(1), \quad S^{1,2} = b_3 z S^{1,1} S^{3,1}(1),$$

$$j = 1, i \geq 2, \quad S^{i,1} = z S^{1,1} S^{i-1,2}(1),$$

$$S^{2,2} = b_3 S^{2,1} S^{3,1}(1) + S^{1,1}(1), \quad S^{3,2} = b_3 z S^{3,1} S^{3,1}(1) + S^{2,1}(1).$$

The functions $f^{i,j}$ satisfy the identities

$$z f^{1,1} - 1 = b_p f^{1,1} f^{p,q}(1),$$

$$i = 1, j \geq 2, \quad f^{1,j} = b_p f^{1,1} f^{p,j-1}(1),$$

$$j = 1, i \geq 2, \quad f^{i,1} = f^{1,1} f^{i-1,q}(1),$$

$$i \geq 2, j \geq 2, \quad f^{i,j} = b_p f^{i,1} f^{p,j-1}(1) + f^{i-1,j-1}(1).$$

Proof. The preceding identities are used. From the classical formulae for the usual product of two series, the results follow. For the functions $f^{i,j}$ the link with the functions $S^{i,j}$ is used and the results follow. \square

5. Matrix Stieltjes continued fraction

For sake of completeness we first recall some definitions and some results of the general theory of matrix continued fractions [13].

5.1. Matrix continued fractions

Matrix continued fractions are an extension of the vector-continued fractions introduced already by Jacobi, and studied by several authors (see for example [6,10]). The notations used here are those of Sorokin and Van Iseghem [13], where the matrices are $p \times q$.

We are interested in a ratio of matrices KH^{-1} , $K \in \mathcal{M}_{p,q}$, $H \in \mathcal{M}_{q,q}$ and as usual an equivalence relation is defined in the set $\mathcal{M}_{p+q,q}$ which is in fact the set of the pairs (H, K) ,

$$A, A' \in \mathcal{M}_{p+q,q}, \quad A \sim A' \Leftrightarrow \exists C \in \mathcal{M}_{q,q}, \det C \neq 0, \quad A' = AC.$$

Let $\mathcal{G}_{p,q}$ be the set of the equivalent classes of matrices (Grassmann space), then operations are defined in $\mathcal{G}_{p,q}$ through the canonical injection from $\mathcal{M}_{p,q}$ to $\mathcal{G}_{p,q}$. Denote by I_q the unit matrix of size $q \times q$, then

$$\pi : \mathcal{M}_{p,q} \rightarrow \mathcal{M}_{p+q,q} \rightarrow \mathcal{G}_{p,q}, \quad A \rightarrow \begin{pmatrix} I_q \\ A \end{pmatrix} \rightarrow \mathcal{C}l \begin{pmatrix} I_q \\ A \end{pmatrix}.$$

We now define what will be used as a quotient in the space $\mathcal{M}_{p,q}$ and will be denoted by $1/Z = T(Z)$. Operators T and \tilde{T} are the same functions defined, respectively, on $\mathcal{M}_{p,q}$ and $\mathcal{M}_{p+q,q}$.

Let \tilde{T} , defined on $\mathcal{M}_{p+q,q}$, be the permutation of the rows which puts the last row at the first place. The operator T is defined from $\mathcal{M}_{p,q}$ to $\mathcal{M}_{p,q}$ and by a straightforward computation we obtain the direct definition of T as a transformation of $\mathcal{M}_{p,q}$ ($T(B)$ is defined if $b_{p,q} \neq 0$):

$$T(B) = \frac{1}{b_{p,q}} \begin{pmatrix} 1 & -b_{p,1} & \cdots & -b_{p,q-1} \\ b_{1,q} & b_{1,1}b_{p,q} - b_{1,q}b_{p,1} & \cdots & b_{1,q-1}b_{p,q} - b_{1,q}b_{p,q-1} \\ \vdots & \vdots & \ddots & \vdots \\ b_{p-1,q} & b_{p-1,1}b_{p,q} - b_{p-1,q}b_{p,1} & \cdots & b_{p-1,q-1}b_{p,q} - b_{p-1,q}b_{p,q-1} \end{pmatrix}. \quad (15)$$

As, clearly $(\tilde{T})^{p+q} = \text{Id}$, \tilde{T} is to be considered as a ‘partial’ quotient and if $p=q$ then $(\tilde{T})^p(A) = A^{-1}$. The previous formula could be taken as a definition.

5.2. Continued fraction associated to the resolvent function

From the recurrence relations written for the functions $f^{i,j}$, we get with $D = 1/f^{1,1} = z - b_p f^{p,q}(1)$, and using the expression of $T(B)$ just recalled (15)

$$\begin{aligned} \begin{pmatrix} f^{1,1} & f^{1,2} \\ f^{2,1} & f^{2,2} \\ f^{3,1} & f^{3,2} \end{pmatrix} &= \frac{1}{D} \begin{pmatrix} 1 & b_3 f^{3,1}(1) \\ f^{1,2}(1) & f^{1,1}(1)D + b_3 f^{1,2}(1)f^{3,1}(1) \\ f^{2,2}(1) & f^{2,1}(1)D + b_3 f^{2,2}(1)f^{3,1}(1) \end{pmatrix} \\ &= \frac{1}{\begin{pmatrix} f^{1,1}(1) & f^{1,2}(1) \\ f^{2,1}(1) & f^{2,2}(1) \\ -b_3 f^{3,1}(1) & z - b_3 f^{3,2}(1) \end{pmatrix}} \\ &= \frac{1}{\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & z \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -b_3 \end{pmatrix}} \begin{pmatrix} f^{1,1}(1) & f^{1,2}(1) \\ f^{2,1}(1) & f^{2,2}(1) \\ f^{3,1}(1) & f^{3,2}(1) \end{pmatrix}. \end{aligned}$$

From this we have the following theorem.

Theorem 5.1. *The resolvent function associated to the operator A has an expansion as a matrix continued fraction*

$$\frac{I_p}{P+} \frac{C_1}{P+} \frac{C_2}{P+\dots},$$

where the parameters of the continued fraction are defined for all n greater than 1 by

$$C_n = \begin{pmatrix} (I_{p-1}) & 0 \\ 0 & -b_{p+n-1} \end{pmatrix}, \quad P = \begin{pmatrix} 0 & \dots & 0 \\ \vdots & \vdots & 0 \\ 0 & \dots & z \end{pmatrix}, \quad P \text{ an } p \times q \text{ matrix.} \tag{16}$$

In other words, we get the recurrence relation

$$F(k) = \frac{1}{P + \text{diag}(\text{diag}(I_{p-1}), -b_{p+k-1})F(k+1)}.$$

If the normalization does not impose $a_n=1$, A has two diagonals a_n and b_n ; genetic sums can also be computed in that case and we would find a continued fraction given by the following recurrence relation:

$$F(k) = \frac{1}{P + \text{diag}(\text{diag}(I_{p-1}), -b_{p+k-1})F(k+1)\text{diag}(\text{diag}(I_{q-1}), a_k)}.$$

In all cases, we obtain an expansion of F in a matrix continued fraction by a generalization of the Jacobi–Perron algorithm [10]. Using this theory [13], we get for the convergent different forms

$$(y_n, \dots, y_{n+q-1}) = \begin{pmatrix} O_n \\ P_n \end{pmatrix} \sim \begin{pmatrix} I_q \\ \Pi_n \end{pmatrix}, \quad \Pi_n = P_n O_n^{-1},$$

where y_n are the columns of size $p+q$ satisfying

$$x y_n = b_n y_{n-p} + a_n y_{n+q}$$

and if $y_n = (H_n, K_n)^t$, and n defines the regular multiindex (n_1, \dots, n_p) , then

$$F H_n - K_n = \left(O \left(\frac{1}{z^{n_1+1}} \right), \dots, O \left(\frac{1}{z^{n_p+1}} \right) \right)^t.$$

6. Zeros, Sturm–Liouville problem

From now on, the parameters a_n and b_n are supposed to be positive, which is equivalent to say that system S is positive.

The proofs are written in the case $p=3, q=2$. By definition we have

$$\Pi_n = \begin{pmatrix} K_n^1 & K_{n+1}^1 \\ K_n^2 & K_{n+1}^2 \\ K_n^3 & K_{n+1}^3 \end{pmatrix} \begin{pmatrix} H_n^1 & H_{n+1}^1 \\ H_n^2 & H_{n+1}^2 \end{pmatrix}^{-1}.$$

Hence, the common denominator is

$$q_n = \det \begin{pmatrix} H_n^1 & H_{n+1}^1 \\ H_n^2 & H_{n+1}^2 \end{pmatrix}.$$

Lemma 6.1. *The following statements hold:*

1. q_n has real coefficients, is of degree n .
2. The leading coefficient of q_n has sign $(-1)^n$.
3. q_n is Z_{p+q} invariant, i.e., $q_n \in \text{Span}\{x^k, k = n \bmod(p + q)\}$.
4. For any positive n , the polynomials $q_{n(p+q)+k}$, $k = 0, \dots, p + q - 1$, have a zero of order k at the point zero.
5. if $x \rightarrow 0$, then $q_n(x) \sim \eta_n(-x)^k$, where $\eta_n > 0$, $n = k \bmod(p + q)$, $k = 0, \dots, p + q - 1$.

Proof. From the recurrence for the H_n , all coefficients are real and from the definition of the basis h_k , H_n^1 is of degree $[n/2]$ as H_n^2 is of degree $k - 1$ if $n = 2k$ and k if $n = 2k + 1$, so the degree of q_n is n .

For the sign of the leading coefficient, we get that $a_{n-1}q_n$ and $x(H_{n-1}^2H_n^1 - H_n^2H_{n-1}^1)$ have the same leading coefficient, so the sign of this leading coefficient is $(-1)^n$, once the initial property is verified. It is the same for the term of lowest degree.

Invariance of q_n follows from invariance of H_n and K_n . It follows also that $q_{n(p+q)+k}$ has a zero of order k at point zero. \square

The following lemma plays the main role for the proof of theorem B.

Lemma 6.2. *The following statements hold:*

1. The polynomials $q_{n(p+q)+k}$, $k = 0, \dots, p + q - 1$ have exactly n positive zeros.
2. The positive zeros of q_n and q_{n+1} interlace.
3. The rational functions $z^{\phi^{i,j}} \Pi_n^{i,j}$ have positive residues at all poles, only some residues at the point $z = 0$ may be equal zero.

Proof. Let us consider

$$\Pi_n^{1,1} = \frac{p_n}{q_n}, \quad p_n = \begin{vmatrix} K_n^1 & K_{n+1}^1 \\ H_n^2 & H_{n+1}^2 \end{vmatrix}.$$

The same investigation holds for the other $\Pi_n^{i,j}$. We consider the determinant

$$\Delta_n = \begin{vmatrix} p_n & p_{n+1} \\ q_n & q_{n+1} \end{vmatrix} = H_{n+1}^2 \begin{vmatrix} K_n^1 & K_{n+1}^1 & K_{n+2}^1 \\ H_n^1 & H_{n+1}^1 & H_{n+2}^1 \\ H_n^2 & H_{n+1}^2 & H_{n+2}^2 \end{vmatrix}.$$

For a polynomial, we write $\text{sgn}(q) = 1$ (respectively -1) if all nonzero coefficients of q are positive (respectively negative). We will prove that $\text{sgn}(\Delta_n) = 1$ for $n \geq 4$.

We first prove, by induction, that $\text{sgn}(H_n^2) = (-1)^{n-1}$.

From the recurrence relation (the same for the K_n), with positive coefficients a_n, b_n

$$xH_n^2 = a_n H_{n+2}^2 + b_n H_{n-3}^2$$

and from the recurrence assumption, we get

$$\text{sgn}(H_n^2) = (-1)^{n-1}, \quad \text{sgn}(H_{n-3}^2) = (-1)^{n-4} \Rightarrow \text{sgn}(H_{n+2}^2) = (-1)^{n+1}.$$

The initial values are checked directly.

Let us denote

$$(n_1 | n_2 | n_3) = \begin{vmatrix} K_{n_1}^1 & K_{n_2}^1 & K_{n_3}^1 \\ H_{n_1}^1 & H_{n_2}^1 & H_{n_3}^1 \\ H_{n_1}^2 & H_{n_2}^2 & H_{n_3}^2 \end{vmatrix}.$$

To prove $\text{sgn}(\Delta_n) = 1$, we have to prove that $\text{sgn}(n | n + 1 | n + 2) = (-1)^n$. By using the recurrence relations for the H_n , we get

$$a_n(n | n + 1 | n + 2) = -b_n(n - 3 | n | n + 1),$$

$$a_{n-1}(n - 3 | n | n + 1) = -x(n - 3 | n - 1 | n) - b_{n-1}(n - 4 | n - 3 | n),$$

$$a_{n-2}(n - 3 | n - 1 | n) = -x(n - 3 | n - 2 | n - 1) - b_{n-2}(n - 5 | n - 3 | n - 1),$$

$$a_{n-2}(n - 4 | n - 3 | n) = x(n - 4 | n - 3 | n - 2) - b_{n-2}(n - 5 | n - 4 | n - 3),$$

$$a_{n-3}(n - 5 | n - 3 | n - 1) = -b_{n-3}(n - 6 | n - 5 | n - 3),$$

$$a_{n-5}(n - 6 | n - 5 | n - 3) = -b_{n-5}(n - 8 | n - 6 | n - 5).$$

The recurrence assumption is taken as

$$\text{sgn}(k | k + 1 | k + 2) = (-1)^k, \quad k < n,$$

$$\text{sgn}(k - 3 | k - 1 | k) = (-1)^k, \quad k < n.$$

Now, taking the preceding equalities from the bottom to the top prove that the recurrence assumption is in fact true for all n , once the initial conditions are satisfied, which is checked directly ($n \geq 4$).

Then $\text{sgn}(n | n + 1 | n + 2) = (-1)^n$, and $\text{sgn}(\Delta_n) = 1$.

We now study the zeros properties of the polynomials \mathbf{q}_n . It is enough to investigate the behaviour of \mathbf{q}_n on the interval $[0, +\infty[$. We have proved that all coefficients of the polynomial Δ_n are nonnegative, as it is not identically zero, then $\Delta_n > 0$ if $x > 0$.

If, for $\xi > 0$, we have $\mathbf{q}_n(\xi) = 0$, then

$$\Delta_{n-1}(\xi) = -\mathbf{p}_n(\xi)\mathbf{q}_{n-1}(\xi) > 0, \tag{17}$$

$$\Delta_n(\xi) = \mathbf{p}_n(\xi)\mathbf{q}_{n+1}(\xi) > 0,$$

so $\mathbf{q}_{n-1}(\xi)$ and $\mathbf{q}_{n+1}(\xi)$ have different signs.

We consider the polynomial q_{5n} , and take as recurrence assumption that q_{5n-1} and q_{5n-2} have $n - 1$ simple positive zeros which interlace. The beginning of the induction is checked directly. Let us denote by ξ_1, \dots, ξ_{n-1} the $n - 1$ positive zeros of q_{5n-1} , written in increasing order. It follows that

$$q_{5n-2}(\xi_1) > 0, \quad q_{5n-2}(\xi_2) < 0, \dots$$

hence $q_{5n}(\xi_1) < 0, q_{5n}(\xi_2) > 0, \dots$, and $q_{5n}(0) > 0$. So q_{5n} has at least one zero on each interval

$$]0, \xi_1[,]\xi_1, \xi_2[, \dots,]\xi_{n-2}, \xi_{n-1}[.$$

By property (2) of the previous lemma, q_{5n} and q_{5n-1} have different signs at infinity, hence q_{5n} has a zero on the interval $]\xi_{n-1}, +\infty[$. Now q_{5n} has at least n positive zeros, but it cannot have more so q_{5n} has n simple positive zeros, which interlace with those of q_{5n-1} .

Let us come now to the polynomials p_n . Similarly they are Z_5 invariant too. If ξ_j^* are the positive zeros of q_{5n} , written in increasing order, then $p_{5n}(\xi_j^*)$ and $q_{5n-1}(\xi_j^*)$ have different signs. So $p_{5n}(\xi_1^*) < 0, p_{5n}(\xi_2^*) > 0, \dots$ and it follows that

$$q'_{5n}(\xi_1^*) < 0, \quad q'_{5n}(\xi_2^*) > 0, \dots$$

hence $p_n(\xi_j^*)$ and $q'_n(\xi_j^*)$ have the same sign, so it follows that the residue at point ξ_j^* , which is $p_n(\xi_j^*)/q'_n(\xi_j^*)$, is positive. The same result is obtained for the other indices. \square

The preceding result can be rewritten in the following form, always with Φ defined in (7).

Lemma 6.3. *For each pair of indices (i, j) , there exists a positive discrete measure such that*

$$z^{\Phi^{i,j}} \Pi_n^{i,j}(z) = \int \frac{d\mu_n^{i,j}(x)}{z - x}. \tag{18}$$

Proof. The measure has mass equal to the residual at each pole of q_n . The residuals being positive, the measure is positive. The support is the same for all (i, j) , as it is the set of zeros of q_n . \square

This result can be written in a matrix form, with some matrix $d\mu_n$ of positive measures

$$z^\Phi \Pi_n(z) = \int \frac{d\mu_n(x)}{z - x}. \tag{19}$$

7. Lax pair

We consider matrix A for the operator of multiple on the variable x in the basis of polynomials $H_n : AH = xH$, where

$$A(e_i) = a_{i-q}e_{i-q} + b_{i+p}a_{i+p}.$$

Matrix A depends on the normalization of the sequence H_n . We will keep the notation A for the monic polynomials H_n^0 , i.e., $a_n = 1$, and call \tilde{A} the generalized Jacobi case, i.e., the a_n and the b_n satisfy (13)

$$(a_n \dots a_{n+p-1})^q = (b_{n+p} \dots b_{n+p+q-1})^p. \tag{20}$$

We are looking for a Lax pair for the matrix A

$$A' = [A, B],$$

which defines the differential equations satisfied by the b_n . As in [1], $B = A_-^{p+q}$ (the lower part of A^{p+q}) gives rise to a matrix $[A, B]$ of the same structure as A' ,

$$A^{p+q}(e_i) = \sum_{k=-q}^p \alpha_{i+k(p+q)}^i e_{i+k(p+q)}, \quad B(e_i) = \sum_{k=1}^p \alpha_{i+k(p+q)}^i e_{i+k(p+q)}.$$

For $k > 1$, the coefficient of $e_{i+k(p+q)+p}$ in $AB(e_i)$ and in $BA(e_i)$ is the coefficient of $e_{i+k(p+q)+p}$ in $A^{p+q+1}(e_i)$, so

$$(AB - BA)(e_i) = (\alpha_{i+p+q}^i - \alpha_{i+p}^{i-q})e_{i+p}$$

and $A' = [A, B]$ is equivalent to the family of differential equations

$$b'_{i+p} = \alpha_{i+p+q}^i - \alpha_{i+p}^{i-q}.$$

For $q = 1$, i.e., the vector case [1], it is $(A(e_i) = e_{i-1} + b_{i+p}e_{i+p})$,

$$\alpha_{i+p}^{i-1} = \sum_{i_1=i}^{i+p-1} b_{i_1} \sum_{i_2=i+p}^{i_1+p} b_{i_2},$$

$$\alpha_{i+p+q}^i - \alpha_{i+p}^{i-q} = b_{i+p} \sum_{i_2=i+p-1}^{i+2p} b_{i_2} + \sum_{i_1=i+1}^{i+p-1} b_{i_1} \left(\sum_{i_2=i+p+1}^{i_1+p} b_{i_2} - \sum_{i_2=i+p}^{i_1+p} b_{i_2} \right) - b_i b_{i+p},$$

$$b'_{i+p} = b_{i+p} \left(\sum_{i_2=i+p+1}^{i+2p} b_{i_2} - \sum_{i_1=i}^{i+p-1} b_{i_1} \right).$$

For $p = 1$, and q any integer [11] $(A(e_i) = e_{i-q} + b_{i+1}e_{i+1})$,

$$B(e_i) = b_{i+1} \cdots b_{i+q+1} e_{i+q+1},$$

$$b'_{i+1} = b_{i+1}(b_{i+2} \cdots b_{i+q+2} - b_i \cdots b_{i-q}).$$

For p and q greater than 1, this gives more complicated formulae. If we write

$$b'_{i+p} = b_{i+p}(U_{i+p} - U_{i-q}),$$

then U_i is a part of a genetic sum, there is at the first level of sum p terms and the final monomials are of degree q . For $p = 3, q = 2$ the equations are

$$b'_{i+3} = b_{i+3}(b_{i+6}(b_{i+9} + b_{i+7} + b_{i+5}) + b_{i+4}(b_{i+7} + b_{i+5}) + b_{i+2}b_{i+5}) - (b_{i+1}(b_{i+4} + b_{i+2} + b_i) + b_{i-1}(b_{i+2} + b_i) + b_{i-3}b_i).$$

We now go to the generalized Jacobi matrix, $\tilde{A}(e_i) = a_{i-q}e_{i-q} + b_{i+p}e_{i+p}$, a_i and b_i satisfying (13). If H_n^0 are the monic polynomials, we consider $H_n = u_n H_n^0$ as defined in Section 3 and define the new parameters

$$a_n = \alpha_n^{p/p+q}, \quad b_{n+p} = \beta_{n+p}^{q/p+q}.$$

In the scalar case, \tilde{A} is symmetric and \tilde{B} must be skew-symmetric, here something of the same kind is recovered, we obtain as a solution for \tilde{B} (for any matrix M_+ and M_- are the upper and lower part of the matrix minus the diagonal),

$$\tilde{B} = \frac{q}{p+q}(\tilde{A}^{p+q})_+ - \frac{p}{p+q}(\tilde{A}^{p+q})_-,$$

$$a'_{i-q} = -\frac{p}{p+q}(b_{i-q}\alpha_{i-p-q}^i - b_{i+p}\alpha_{i-q}^{i+p}) = -\frac{p}{p+q}a_{i-q}(V_{i-q} - V_{i-p-2q}),$$

$$b'_{i+p} = \frac{q}{p+q}(a_{i+p}\alpha_{i+p+q}^i - a_{i-q}\alpha_{i+p}^{i-q}) = \frac{q}{p+q}b_{i+p}(U_{i+p} - U_{i-q}).$$

As the a_n and the b_n are linked by (13), both equations are equivalent up to a change of variable. We first write the equations in a and b , then in α and β which are the dual forms of the same equation. The equation in β is exactly the same as the equation obtained in the first case with the matrix A associated to the unitary polynomials.

The final results in the case $p = 3, q = 2$ are

$$b'_{i+3} = \frac{2}{5}b_{i+3}(U_{i+3} - U_{i-2}),$$

$$U_i = a_{i+3}(b_{i+6}(b_{i+9}a_{i+7}a_{i+5} + a_{i+4}(b_{i+7}a_{i+5} + a_{i+2}b_{i+5})) + a_{i+1}(b_{i+4}(b_{i+7}a_{i+5} + a_{i+2}b_{i+5}) + a_{i-1}b_{i+2}b_{i+5})),$$

$$a'_{i-2} = -\frac{3}{5}a_{i-2}(V_{i-2} - V_{i-7}),$$

$$V_{i-2} = b_{i+3}(b_{i+6}a_{i+4}a_{i+2}a_i + a_{i+1}(b_{i+4}a_{i+2}a_i + a_{i-1}(b_{i+2}a_i + a_{i-3}b_i))).$$

If these equations are written in terms of α_n , and β_n we have $a_n^{5/3} = c_n c_{n+1} = \alpha_n$ and $b_n^{5/2} = c_n c_{n+1} c_{n+2} = \beta_{n+3}$, then we get

$$\begin{aligned} \alpha'_n &= \alpha_n \left(\frac{5}{3} \frac{\alpha'_n}{\alpha_n} \right) & \beta'_{n+3} &= \beta_{n+3} \left(\frac{5}{2} \frac{\beta'_{n+3}}{\beta_{n+3}} \right) \\ &= \alpha_n(V_n - V_{n-5}), & &= \beta_{n+3}(U_{n+3} - U_{n-2}). \end{aligned}$$

The V and U are computed in terms of c_k , then in terms of α and β , and we finally get

$$\alpha'_n = \alpha_n(V_n - V_{n-5}),$$

$$V_n = \alpha_{n+2}(\alpha_{n+4}(\alpha_{n+6} + \alpha_{n+3}) + \alpha_{n+1}\alpha_{n+3}) + \alpha_{n-1}\alpha_{n+1}\alpha_{n+3},$$

$$\beta'_{n+3} = \beta_{n+3}(U_{n+3} - U_{n-2}),$$

$$U_{n+3} = \beta_{n+6}(\beta_{n+9} + \beta_{n+7} + \beta_{n+5}) + \beta_{n+4}(\beta_{n+7} + \beta_{n+5}) + \beta_{n+2}\beta_{n+5}.$$

8. Dynamical systems

Consider the moment problem dealing with a positive sequence S . Φ still defined by (7), let us denote

$$\Delta_\rho = \bigcup_{k=1}^{p+q} [0, \zeta^k \rho], \quad \zeta = \exp\left(\frac{2i\pi}{p+q}\right), \quad \Delta = \Delta_\infty.$$

Lemma 8.1. 1. *If S is positive, then there exists a matrix of positive Borel measures with common support on Δ :*

$$d\mu = (d\mu^{k,j}), \quad k = 1, \dots, p, \quad j = 1, \dots, q$$

such that

$$z^{\Phi^{k,j}} f^{k,j}(z) = \int_{\Delta} \frac{d\mu^{k,j}(x)}{z-x}.$$

2. *The matrix is bounded, if and only if, the measure $d\mu$ has a compact support. In this case, the measure is uniquely defined.*

3. *If matrix A is bounded, then the generalization of Markov theorem holds: the sequence of approximants Π_n converges to F on compact sets of the domain $D = \bar{C} - \Delta_\rho$, for some constant ρ .*

Proof. In Section 6, we have proved that for each pair of indices k, j , the rational functions $\Pi_n^{k,j}$ can be decomposed into elementary elements:

$$z^{\Phi^{k,j}} \Pi_n^{k,j}(z) = \int_{\Delta} \frac{d\mu_n^{k,j}(x)}{z-x}, \tag{21}$$

where $d\mu_n^{k,j}$ are discrete positive measures with common support in the set of the zeros of the polynomial q_n . In matrix form

$$z^\Phi \Pi_n(z) = \int_{\Delta} \frac{d\mu_n(x)}{z-x}.$$

It means that $d\mu_n$ is the solution of the finite moment problem

$$\int_{\Delta} x^{(p+q)v} d\mu_n(x) = S_v, \quad v = 0, \dots, N_n$$

with $N_n \rightarrow \infty$. By the first Helly theorem, it is possible to choose a weak converging subsequence, i.e., $(d\mu_n)_{n \in A}$.

By the second Helly theorem, the limit measure $d\mu$ is a solution of the full moment problem

$$\int_{\Delta} x^{(p+q)v} d\mu(x) = S_v, \quad v \geq 0,$$

that is the same as

$$z^\Phi F(z) = \int_{\Delta} \frac{d\mu(x)}{z-x}.$$

Let us now prove the second point of the lemma. From the genetic sums, it follows that A is bounded if and only if the moments S_n have a geometric estimation. This fact is, as well known,

equivalent to the compactness of the spectrum. The uniqueness of the solution follows from the uniqueness theorem for holomorphic functions.

For the last point of the theorem: let ρ be the minimal radius of the disk including the support of $d\mu$. The proof of the Markov theorem is standard. From (21), follows the uniform boundness of the sequence (Π_n) on compact sets of the domain D . By Montel’s theorem, the sequence (Π_n) is compact. Because it converges to F for the archimedian norm, and ∞ is in D , F is the unique limit point of (Π_n) . Hence (Π_n) converges to F on compact sets of D . \square

Remark 8.2. The measure $d\mu$ is the spectral measure of the operator A . If we know $d\mu$, we can construct the operator A by decomposition of F into a continued fraction. Note that the arbitrary measure $d\mu$ does not have positive moments. For example, it is necessary that all elements of the matrix $d\mu$ have a common support. But this condition is not sufficient. There exist some sufficient conditions and examples.

Remark 8.3. The support of $d\mu$ is only a subset of the spectrum of the operator A , and the constant ρ is less than the spectrum radius of the operator.

Let us consider the case $p=3, q=2$. By initial data $b_{n+3}(0)$ we construct the operator A and solve the direct spectral problem, i.e., we look for the measure $d\mu$ by summing the continued fraction.

Consider the special dynamics of the spectral measure

$$d\tilde{\mu}(x, t) = \exp(x^5 t) d\mu(x), \quad \tilde{S}_0^{1,1}(t) = \int_A d\tilde{\mu}^{1,1}(x, t), \quad d\mu(x, t) = \frac{d\tilde{\mu}(x, t)}{\tilde{S}_0^{1,1}(t)},$$

then

$$d(\tilde{\mu})' = x^5 d\tilde{\mu}.$$

Hence the power moments \tilde{S}_n of the measure $d\tilde{\mu}$ satisfy the following differential equation:

$$(\tilde{S}_n)' = \tilde{S}_{n+1}.$$

Because the power moments of the measure $d\mu$ are $S_n = \tilde{S}_n / \tilde{S}_0^{1,1}$, then

$$\begin{aligned} S_n' &= \frac{\tilde{S}_n'}{\tilde{S}_0^{1,1}} - \tilde{S}_n \frac{(\tilde{S}_0^{1,1})'}{(\tilde{S}_0^{1,1})^2} = \frac{\tilde{S}_{n+1}}{\tilde{S}_0^{1,1}} - \frac{\tilde{S}_n}{\tilde{S}_0^{1,1}} \frac{\tilde{S}_1^{1,1}}{\tilde{S}_0^{1,1}} \\ &= S_{n+1} - S_n S_1^{1,1}. \end{aligned}$$

We have proved that this last equation is equivalent to the dynamical system. Thus, the reconstruction parameters $b_{n+3}(t)$ is the inverse spectral problem and its solution is the decomposition of

$$\frac{1}{z^\Phi} \int_A \frac{d\mu(x, t)}{z - x}$$

in a continued fraction.

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Numerical analysis of the non-uniform sampling problem [☆]

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Abstract

We give an overview of recent developments in the problem of reconstructing a band-limited signal from nonuniform sampling from a numerical analysis view point. It is shown that the appropriate design of the finite-dimensional model plays a key role in the numerical solution of the nonuniform sampling problem. In the one approach (often proposed in the literature) the finite-dimensional model leads to an ill-posed problem even in very simple situations. The other approach that we consider leads to a well-posed problem that preserves important structural properties of the original infinite-dimensional problem and gives rise to efficient numerical algorithms. Furthermore, a fast multilevel algorithm is presented that can reconstruct signals of unknown bandwidth from noisy nonuniformly spaced samples. We also discuss the design of efficient regularization methods for ill-conditioned reconstruction problems. Numerical examples from spectroscopy and exploration geophysics demonstrate the performance of the proposed methods. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

The problem of reconstructing a signal f from nonuniformly spaced measurements $f(t_j)$ arises in areas as diverse as geophysics, medical imaging, communication engineering, and astronomy. A successful reconstruction of f from its samples $f(t_j)$ requires a priori information about the signal, otherwise the reconstruction problem is ill-posed. This a priori information can often be obtained from physical properties of the process generating the signal. In many of the aforementioned applications the signal can be assumed to be (essentially) band-limited.

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Recall that a signal (function) is band-limited with bandwidth Ω if it belongs to the space \mathbf{B}_Ω , given by

$$\mathbf{B}_\Omega = \{f \in L^2(\mathbb{R}): \hat{f}(\omega) = 0 \text{ for } |\omega| > \Omega\}, \quad (1)$$

where \hat{f} is the Fourier transform of f defined by

$$\hat{f}(\omega) = \int_{-\infty}^{+\infty} f(t)e^{-2\pi i\omega t} dt.$$

For convenience and without loss of generality we restrict our attention to the case $\Omega = \frac{1}{2}$, since any other bandwidth can be reduced to this case by a simple dilation. Therefore, we will henceforth use the symbol \mathbf{B} for the space of band-limited signals.

It is now more than 50 years ago that Shannon published his celebrated sampling theorem [35]. His theorem implies that any signal $f \in \mathbf{B}$ can be reconstructed from its regularly spaced samples $\{f(n)\}_{n \in \mathbb{Z}}$ by

$$f(t) = \sum_{n \in \mathbb{Z}} f(n) \frac{\sin \pi(t - n)}{\pi(t - n)}. \quad (2)$$

In practice, however, we seldom enjoy the luxury of equally spaced samples. The solution of the nonuniform sampling problem poses much more difficulties, the crucial questions being:

- Under which conditions is a signal $f \in \mathbf{B}$ uniquely defined by its samples $\{f(t_j)\}_{j \in \mathbb{Z}}$?
- How can f be stably reconstructed from its samples $f(t_j)$?

These questions have led to a vast literature on nonuniform sampling theory with deep mathematical contributions see [11,25,3,6,15] to mention only a few. There is also no lack of methods claiming to efficiently reconstruct a function from its samples [42,41,1,14,40,26,15]. These numerical methods naturally have to operate in a finite-dimensional model, whereas theoretical results are usually derived for the infinite-dimensional space \mathbf{B} . From a numerical point of view the “reconstruction” of a band-limited signal f from a finite number of samples $\{f(t_j)\}_{j=1}^r$ amounts to computing an approximation to f (or \hat{f}) at sufficiently dense (regularly) spaced grid points in an interval (t_1, t_r) .

Hence in order to obtain a “complete” solution of the sampling problem following questions have to be answered:

- Does the approximation computed within the finite-dimensional model actually converge to the original signal f , when the dimension of the model approaches infinity?
- Does the finite-dimensional model give rise to fast and stable numerical algorithms?

These are the questions that we have in mind, when presenting an overview on recent advances and new results in the nonuniform sampling problem from a numerical analysis view point.

In Section 2 it is demonstrated that the celebrated frame approach does only lead to fast and stable numerical methods when the finite-dimensional model is carefully designed. The approach usually proposed in the literature leads to an ill-posed problem even in very simple situations. We discuss several methods to stabilize the reconstruction algorithm in this case. In Section 3 we derive an alternative finite-dimensional model, based on trigonometric polynomials. This approach leads to a well-posed problem that preserves important structural properties of the original infinite-dimensional problem and gives rise to efficient numerical algorithms. Section 4 describes how this approach

can be modified in order to reconstruct band-limited signals for the in practice very important case when the bandwidth of the signal is not known. Furthermore, we present regularization techniques for ill-conditioned sampling problems. Finally Section 5 contains numerical experiments from spectroscopy and geophysics.

Before we proceed we introduce some notation that will be used throughout the paper. If not otherwise mentioned $\|h\|$ always denotes the $L^2(\mathbb{R})$ -norm ($\ell^2(\mathbb{Z})$ -norm) of a function (vector). For operators (matrices) $\|T\|$ is the standard operator (matrix) norm. The condition number of an invertible operator T is defined by $\kappa(A) = \|A\| \|A^{-1}\|$ and the spectrum of T is $\sigma(T)$. I denotes the identity operator.

1.1. Nonuniform sampling, frames, and numerical algorithms

The concept of frames is an excellent tool to study nonuniform sampling problems [13,2,1,24,15,44]. The frame approach has the advantage that it gives rise to deep theoretical results and also to the construction of efficient numerical algorithms – if (and this point is often ignored in the literature) the finite-dimensional model is properly designed.

Following Duffin and Schaeffer [11], a family $\{f_j\}_{j \in \mathbb{Z}}$ in a separable Hilbert space \mathbf{H} is said to be a frame for \mathbf{H} , if there exist constants (the *frame bounds*) $A, B > 0$ such that

$$A\|f\|^2 \leq \sum_j |\langle f, f_j \rangle|^2 \leq B\|f\|^2, \quad \forall f \in \mathbf{H}. \tag{3}$$

We define the *analysis operator* T by

$$T : f \in \mathbf{H} \rightarrow Tf = \{\langle f, f_j \rangle\}_{j \in \mathbb{Z}} \tag{4}$$

and the *synthesis operator*, which is just the adjoint operator of T , by

$$T^* : c \in \ell^2(\mathbb{Z}) \rightarrow T^*c = \sum_j c_j f_j. \tag{5}$$

The *frame operator* S is defined by $S = T^*T$, hence $Sf = \sum_j \langle f, f_j \rangle f_j$. S is bounded by $AI \leq S \leq BI$ and hence invertible on \mathbf{H} .

We will also make use of the operator TT^* in form of its Gram matrix representation $R : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$ with entries $R_{j,l} = \langle f_j, f_l \rangle$. On $\mathcal{R}(T) = \mathcal{R}(R)$ the matrix R is bounded by $AI \leq R \leq BI$ and invertible. On $\ell^2(\mathbb{Z})$ this inverse extends to the *Moore–Penrose inverse* or pseudo-inverse R^+ (cf. [12]).

Given a frame $\{f_j\}_{j \in \mathbb{Z}}$ for \mathbf{H} , any $f \in \mathbf{H}$ can be expressed as

$$f = \sum_{j \in \mathbb{Z}} \langle f, f_j \rangle \gamma_j = \sum_{j \in \mathbb{Z}} \langle f, \gamma_j \rangle f_j, \tag{6}$$

where the elements $\gamma_j := S^{-1}f_j$ form the so-called dual frame and the frame operator induced by γ_j coincides with S^{-1} . Hence if a set $\{\gamma_j\}_{j \in \mathbb{Z}}$ establishes a frame for \mathbf{H} , we can reconstruct any function $f \in \mathbf{H}$ from its moments $\langle f, f_j \rangle$.

One possibility to connect sampling theory to frame theory is by means of the *sinc*-function

$$\text{sinc}(t) = \frac{\sin \pi t}{\pi t}. \tag{7}$$

Its translates give rise to a *reproducing kernel* for \mathbf{B} via

$$f(t) = \langle f, \text{sinc}(\cdot - t) \rangle \quad \forall t, f \in \mathbf{B}. \tag{8}$$

Combining (8) with formulas (3) and (6) we obtain following well-known result [13,2].

Theorem 1.1. *If the set $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ is a frame for \mathbf{B} , then the function $f \in \mathbf{B}$ is uniquely defined by the sampling set $\{f(t_j)\}_{j \in \mathbb{Z}}$. In this case we can recover f from its samples by*

$$f(t) = \sum_{j \in \mathbb{Z}} f(t_j) \gamma_j, \quad \text{where } \gamma_j = S^{-1} \text{sinc}(\cdot - t_j), \tag{9}$$

or equivalently by

$$f(t) = \sum_{j \in \mathbb{Z}} c_j \text{sinc}(t - t_j), \quad \text{where } Rc = b \tag{10}$$

with R being the frame Gram matrix with entries $R_{j,l} = \text{sinc}(t_j - t_l)$ and $b = \{b_j\} = \{f(t_j)\}$.

The challenge is now to find easy-to-verify conditions for the sampling points t_j such that $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ (or equivalently the exponential system $\{e^{2\pi i t_j \omega}\}_{j \in \mathbb{Z}}$) is a frame for \mathbf{B} . This is a well-traversed area (at least for one-dimensional signals), and the reader should consult [1,15,24] for further details and references. If not otherwise mentioned from now on we will assume that $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ is a frame for \mathbf{B} .

Of course, neither of formulas (9) and (10) can be actually implemented on a computer, because both involve the solution of an infinite-dimensional operator equation, whereas in practice we can only compute a finite-dimensional approximation. Although the design of a valid finite-dimensional model poses severe mathematical challenges, this step is often neglected in theoretical but also in numerical treatments of the nonuniform sampling problem. We will see, in the sequel, that the way we design our finite-dimensional model is crucial for the stability and efficiency of the resulting numerical reconstruction algorithms.

In the next two sections we describe two different approaches for obtaining finite-dimensional approximations to formulas (9) and (10). The first and more traditional approach, discussed in Section 2, applies a finite section method to Eq. (10). This approach leads to an ill-posed problem involving the solution of a large unstructured linear system of equations. The second approach, outlined in Section 3, constructs a finite model for the operator equation in (9) by means of trigonometric polynomials. This technique leads to a well-posed problem that is tied to efficient numerical algorithms.

2. Truncated frames lead to ill-posed problems

According to Eq. (10) we can reconstruct f from its sampling values $f(t_j)$ via $f(t) = \sum_{j \in \mathbb{Z}} c_j \text{sinc}(t - t_j)$, where $c = R^+ b$ with $b_j = f(t_j)$, $j \in \mathbb{Z}$. In order to compute a finite-dimensional approximation to $c = \{c_j\}_{j \in \mathbb{Z}}$ we use the finite section method [17]. For $x \in \ell^2(\mathbb{Z})$ and $n \in \mathbb{N}$ we define the orthogonal projection P_n by

$$P_n x = (\dots, 0, 0, x_{-n}, x_{-n+1}, \dots, x_{n-1}, x_n, 0, 0, \dots) \tag{11}$$

and identify the image of P_n with the space \mathbb{C}^{2n+1} . Setting $R_n = P_n R P_n$ and $b^{(n)} = P_n b$, we obtain the n th approximation $c^{(n)}$ to c by solving

$$R_n c^{(n)} = b^{(n)}. \tag{12}$$

It is clear that using the truncated frame $\{\text{sinc}(\cdot - t_j)\}_{j=-n}^n$ in (10) for an approximate reconstruction of f leads to the same system of equations.

If $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ is an exact frame (i.e., a Riesz basis) for \mathbf{B} then we have following well-known result.

Lemma 2.1. *Let $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ be an exact frame for \mathbf{B} with frame bounds A, B and $Rc = b$ and $R_n c^{(n)} = b^{(n)}$ as defined above. Then R_n^{-1} converges strongly to R^{-1} and hence $c^{(n)} \rightarrow c$ for $n \rightarrow \infty$.*

Since the proof of this result given in [9] is somewhat lengthy we include a rather short proof here.

Proof. Note that R is invertible on $\ell^2(\mathbb{Z})$ and $A \leq R \leq B$. Let $x \in \mathbb{C}^{2n+1}$ with $\|x\| = 1$, then $\langle R_n x, x \rangle = \langle P_n R P_n x, x \rangle = \langle R x, x \rangle \geq A$. In the same way we get $\|R_n\| \leq B$, hence the matrices R_n are invertible and uniformly bounded by $A \leq R_n \leq B$ and

$$\frac{1}{B} \leq R_n^{-1} \leq \frac{1}{A} \quad \text{for all } n \in \mathbb{N}.$$

The lemma of Kantorovich [32] yields that $R_n^{-1} \rightarrow R^{-1}$ strongly. \square

If $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ is a nonexact frame for \mathbf{B} the situation is more delicate. Let us consider following situation.

Example 1. Let $f \in \mathbf{B}$ and let the sampling points be given by $t_j = j/m$, $j \in \mathbb{Z}$, $1 < m \in \mathbb{N}$, i.e., the signal is regularly oversampled at m times the Nyquist rate. In this case the reconstruction of f is trivial, since the set $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ is a tight frame with frame bounds $A = B = m$. Shannon’s Sampling Theorem implies that f can be expressed as $f(t) = \sum_{j \in \mathbb{Z}} c_j \text{sinc}(t - t_j)$ where $c_j = f(t_j)/m$ and the numerical approximation is obtained by truncating the summation, i.e.,

$$f_n(t) = \sum_{j=-n}^n \frac{f(t_j)}{m} \text{sinc}(t - t_j).$$

Using the truncated frame approach one finds that R is a Toeplitz matrix with entries

$$R_{j,l} = \frac{\sin(\pi/m)(j - l)}{(\pi/m)(j - l)}, \quad j, l \in \mathbb{Z},$$

in other words, R_n coincides with the prolate matrix [36,39]. The unpleasant numerical properties of the prolate matrix are well-documented. In particular, we know that the singular values λ_n of R_n cluster around 0 and 1 with $\log n$ singular values in the transition region. Since the singular values of R_n decay exponentially to zero the finite-dimensional reconstruction problem has become *severely ill-posed* [12], although the infinite-dimensional problem is “perfectly posed” since the frame operator satisfies $S = mI$, where I is the identity operator.

Of course, the situation does not improve when we consider nonuniformly spaced samples. In this case it follows from standard linear algebra that $\sigma(R) \subseteq \{0 \cup [A, B]\}$, or expressed in words, the singular values of R are bounded away from zero. However for the truncated matrices R_n we have

$$\sigma(R_n) \subseteq \{(0, B]\}$$

and the smallest of the singular values of R_n will go to zero for $n \rightarrow \infty$, see [23].

Let $A = U\Sigma V^*$ be the singular value decomposition of a matrix A with $\Sigma = \text{diag}(\{\lambda_k\})$. Then the Moore–Penrose inverse of A is $A^+ = V\Sigma^+U^*$, where (see, e.g., [18])

$$\Sigma^+ = \text{diag}(\{\lambda_k^+\}), \quad \lambda_k^+ = \begin{cases} 1/\lambda_k & \text{if } \lambda_k \neq 0, \\ 0 & \text{otherwise.} \end{cases} \tag{13}$$

For $R_n = U_n \Sigma_n V_n$ this means that the singular values close to zero will give rise to extremely large coefficients in R_n^+ . In fact, $\|R_n^+\| \rightarrow \infty$ for $n \rightarrow \infty$ and consequently $c^{(n)}$ does not converge to c .

Practically, $\|R_n^+\|$ is always bounded due to finite precision arithmetics, but it is clear that it will lead to meaningless results for large n . If the sampling values are perturbed due to round-off error or data error, then those error components which correspond to small singular values λ_k are amplified by the (then large) factors $1/\lambda_k$. Although for a given R_n these amplifications are theoretically bounded, they may be practically unacceptable large.

Such phenomena are well known in regularization theory [12]. A standard technique to compute a stable solution for an ill-conditioned system is to use a truncated singular value decomposition (TSVD) [12]. This means in our case we compute a regularized pseudo-inverse $R_n^{+,\tau} = V_n \Sigma_n^{+,\tau} U_n^*$ where

$$\Sigma_n^{+,\tau} = \text{diag}(\{d_k^+\}), \quad d_k^+ = \begin{cases} 1/\lambda_k & \text{if } \lambda_k \geq \tau, \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

In [23] it is shown that for each n we can choose an appropriate truncation level τ such that the regularized inverses $R_n^{+,\tau}$ converge strongly to R^+ for $n \rightarrow \infty$ and consequently $\lim_{n \rightarrow \infty} \|f - f^{(n)}\| = 0$, where

$$f^{(n)}(t) = \sum_{j=-n}^n c_j^{(n,\tau)} \text{sinc}(t - t_j)$$

with

$$c^{(n,\tau)} = R_n^{+,\tau} b^{(n)}.$$

The optimal truncation level τ depends on the dimension n , the sampling geometry, and the noise level. Thus it is not known a priori and has in principle to be determined for each n independently.

Since τ is of vital importance for the quality of the reconstruction, but no theoretical explanations for the choice of τ are given in the sampling literature, we briefly discuss this issue. For this purpose we need some results from regularization theory.

2.1. Estimation of regularization parameter

Let $Ax = y^\delta$ be given where A is ill-conditioned or singular and y^δ is a perturbed right-hand side with $\|y - y^\delta\| \leq \delta \|y\|$. Since in our sampling problem the matrix under consideration is symmetric,

we assume for convenience that A is symmetric. From a numerical point of view ill-conditioned systems behave like singular systems and additional information is needed to obtain a satisfactory solution to $Ax = y$. This information is usually stated in terms of “smoothness” of the solution x . A standard approach to qualitatively describe smoothness of x is to require that x can be represented in the form $x = Sz$ with some vector z of reasonable norm, and a “smoothing” matrix S , cf. [12,29]. Often it is useful to construct S directly from A by setting

$$S = A^p, \quad p \in \mathbb{N}_0. \tag{15}$$

Usually, p is assumed to be fixed, typically at $p = 1$ or 2 .

We compute a regularized solution to $Ax = y^\delta$ via a truncated SVD and want to determine the optimal regularization parameter (i.e., truncation level) τ .

Under the assumption that

$$x = Sz, \quad \|Ax - y^\delta\| \leq \Delta \|z\|, \tag{16}$$

it follows from Theorem 4.1 in [29] that the optimal regularization parameter τ for the TSVD is

$$\hat{\tau} = \left(\frac{\gamma_1 \delta}{\gamma_2 p} \right)^{1/(p+1)}, \tag{17}$$

where $\gamma_1 = \gamma_2 = 1$ (see [29, Section 6]).

However z and Δ are in general not known. Using $\|Ax - y^\delta\| \leq \delta \|y\|$ and $\|y\| = \|Ax\| = \|ASz\| = \|A^{p+1}z\|$ we obtain $\|y\| \leq \|A\|^{p+1} \|z\|$. Furthermore, setting $\delta \|y\| = \Delta \|z\|$ implies

$$\Delta \leq \delta \|A\|^{p+1}. \tag{18}$$

Hence combining (17) and (18) we get

$$\hat{\tau} \leq \left(\frac{\delta \|A\|^{p+1}}{p} \right)^{1/(p+1)} = \|A\| \left(\frac{\delta}{p} \right)^{1/(p+1)}. \tag{19}$$

Applying these results to solving $R_n c^{(n)} = b^{(n)}$ via TSVD as described in the previous section, we get

$$\hat{\tau} \leq \|R_n\| \left(\frac{\delta}{p} \right)^{1/(p+1)} \leq \|R\| \left(\frac{\delta}{p} \right)^{1/(p+1)} = B \left(\frac{\delta}{p} \right)^{1/(p+1)}, \tag{20}$$

where B is the upper frame bound. Fortunately, estimates for the upper frame bound are much easier to obtain than estimates for the lower frame bound.

Thus using the standard setting $p = 1$ or 2 a good choice for the regularization parameter τ is

$$\tau \subseteq [B(\delta/2)^{1/3}, B(\delta)^{1/2}]. \tag{21}$$

Extensive numerical simulations confirm this choice, see also Section 5.

For instance for the reconstruction problem of Example 1 with noise-free data and machine precision $\varepsilon = \delta = 10^{-16}$, formula (21) implies $\tau \subseteq [10^{-6}, 10^{-8}]$. This coincides very well with numerical experiments.

If the noise level δ is not known, it has to be estimated. This difficult problem will not be discussed here. The reader is referred to [29] for more details.

Although we have arrived now at an implementable algorithm for the nonuniform sampling problem, the disadvantages of the approach described in the previous section are obvious. In general, the

matrix R_n does not have any particular structure, thus the computational costs for the singular value decomposition are $\mathcal{O}(n^3)$ which is prohibitive large in many applications. It is definitely not a good approach to transform a well-posed infinite-dimensional problem into an ill-posed finite-dimensional problem for which a stable solution can only be computed by using a “heavy regularization machinery”.

The methods in [40–42,33,2] coincide with or are essentially equivalent to the truncated frame approach, therefore they suffer from the same instability problems and the same numerical inefficiency.

2.2. CG and regularization of the truncated frame method

As mentioned above one way to stabilize the solution of $R_n c^{(n)} = b^{(n)}$ is a truncated singular value decomposition, where the truncation level serves as regularization parameter. For large n the costs of the singular value decomposition become prohibitive for practical purposes.

We propose the conjugate gradient method [18] to solve $R_n c^{(n)} = b^{(n)}$. It is in general much more efficient than a TSVD (or Tikhonov regularization as suggested in [40]), and at the same time it can also be used as a regularization method.

The standard error analysis for CG cannot be used in our case, since the matrix is ill-conditioned. Rather we have to resort to the error analysis developed in [28,22].

When solving a linear system $Ax = y$ by CG for noisy data y^δ following happens. The iterates x_k of CG may diverge for $k \rightarrow \infty$, however the error propagation remains limited in the beginning of the iteration. The quality of the approximation therefore depends on how many iterative steps can be performed until the iterates turn to diverge. The idea is now to stop the iteration at about the point where divergence sets in. In other words, the iterations count is the regularization parameter which remains to be controlled by an appropriate stopping rule [27,22].

In our case assume $\|b^{(n,\delta)} - b^{(n)}\| \leq \delta \|b^{(n)}\|$, where $b_j^{(n,\delta)}$ denotes a noisy sample. We terminate the CG iterations when the iterates $(c^{(n,\delta)})_k$ satisfy for the first time [22]

$$\|b^{(n)} - (c^{(n,\delta)})_k\| \leq \tau \delta \|b^{(n)}\| \tag{22}$$

for some fixed $\tau > 1$.

It should be noted that one can construct “academic” examples where this stopping rule does not prevent CG from diverging, see [22], “most of the time” however it gives satisfactory results. We refer the reader to [27,22] for a detailed discussion of various stopping criteria.

There is a variety of reasons, besides the ones we have already mentioned, that make the conjugate gradient method and the nonuniform sampling problem a “perfect couple”. See Sections 3, 4.1, and 4.2 for more details.

By combining the truncated frame approach with the conjugate gradient method (with appropriate stopping rule) we finally arrive at a reconstruction method that is of some practical relevance. However, the only existing method at the moment that can handle large scale reconstruction problems seems to be the one proposed in the next section.

3. Trigonometric polynomials and efficient signal reconstruction

In the previous section we have seen that the naive finite-dimensional approach via truncated frames is not satisfactory, it already leads to severe stability problems in the ideal case of regular oversampling. In this section we propose a different finite-dimensional model, which resembles much better the structural properties of the sampling problem, as can be seen below.

The idea is simple. In practice, only a finite number of samples $\{f(t_j)\}_{j=1}^r$ is given, where without loss of generality we assume $-M \leq t_1 < \dots < t_r \leq M$ (otherwise we can always re-normalize the data). Since no data of f are available from outside this region we focus on a local approximation of f on $[-M, M]$. We extend the sampling set periodically across the boundaries, and identify this interval with the (properly normalized) torus \mathbb{T} . To avoid technical problems at the boundaries in the sequel we will choose the interval somewhat larger and consider either $[-M - 1/2, M + 1/2]$ or $[-N, N]$ with $N = M + M/(r - 1)$. For theoretical considerations the choice $[-M - 1/2, M + 1/2]$ is more convenient.

Since the dual group of the torus \mathbb{T} is \mathbb{Z} , periodic band-limited functions on \mathbb{T} reduce to trigonometric polynomials (of course, technically f does then no longer belong to \mathbf{B} since it is no longer in $L^2(\mathbb{R})$). This suggests to use trigonometric polynomials as a realistic finite-dimensional model for a numerical solution of the nonuniform sampling problem. We consider the space \mathbf{P}_M of trigonometric polynomials of degree M of the form

$$p(t) = (2M + 1)^{-1} \sum_{k=-M}^M a_k e^{2\pi i k t / (2M+1)}. \tag{23}$$

The norm of $p \in \mathbf{P}_M$ is

$$\|p\|^2 = \int_{-N}^N |p(t)|^2 dt = \sum_{k=-M}^M |a_k|^2.$$

Since the distributional Fourier transform of p is $\hat{p} = (2M + 1)^{-1} \sum_{k=-M}^M a_k \delta_{k/(2M+1)}$ we have $\text{supp } \hat{p} \subseteq \{k/(2M + 1), |k| \leq M\} \subseteq [-\frac{1}{2}, \frac{1}{2}]$. Hence \mathbf{P}_M is indeed a natural finite-dimensional model for \mathbf{B} .

In general the $f(t_j)$ are not the samples of a trigonometric polynomial in \mathbf{P}_M , moreover the samples are usually perturbed by noise, hence we may not find a $p \in \mathbf{P}_M$ such that $p(t_j) = b_j = f(t_j)$. We therefore consider the least-squares problem

$$\min_{p \in \mathbf{P}_M} \sum_{j=1}^r |p(t_j) - b_j|^2 w_j. \tag{24}$$

Here the $w_j > 0$ are user-defined weights, which can be chosen for instance to compensate for irregularities in the sampling geometry [14].

By increasing M so that $r \leq 2M + 1$ we can certainly find a trigonometric polynomial that interpolates the given data exactly. However in the presence of noise, such a solution is usually rough and highly oscillating and may poorly resemble the original signal. We will discuss the question of the optimal choice of M if the original bandwidth is not known and in presence of noisy data in Section 4.2.

The following theorem provides an efficient numerical reconstruction algorithm. It is also the key for the analysis of the relation between the finite-dimensional approximation in \mathbf{P}_M and the solution of the original infinite-dimensional sampling problem in \mathbf{B} .

Theorem 3.1 (and Algorithm [19,14]). *Given the sampling points $-M \leq t_1 < \dots, t_r \leq M$, samples $\{b_j\}_{j=1}^r$, positive weights $\{w_j\}_{j=1}^r$ with $2M + 1 \leq r$.*

Step 1: Compute the $(2M + 1) \times (2M + 1)$ Toeplitz matrix T_M with entries

$$(T_M)_{k,l} = \frac{1}{2M + 1} \sum_{j=1}^r w_j e^{-2\pi i(k-l)t_j/(2M+1)} \quad \text{for } |k|, |l| \leq M \tag{25}$$

and $y_M \in \mathbb{C}^{(2M+1)}$ by

$$(y_M)_k = \frac{1}{\sqrt{2M + 1}} \sum_{j=1}^r b_j w_j e^{-2\pi i k t_j / (2M+1)} \quad \text{for } |k| \leq M. \tag{26}$$

Step 2: Solve the system

$$T_M a_M = y_M. \tag{27}$$

Step 3: Then the polynomial $p_M \in \mathbf{P}_M$ that solves (24) is given by

$$p_M(t) = \frac{1}{\sqrt{2M + 1}} \sum_{k=-M}^M (a_M)_k e^{2\pi i k t / (2M+1)}. \tag{28}$$

Numerical Implementation of Theorem/Algorithm 3.1.

Step 1: The entries of T_M and y_M of Eqs. (25) and (26) can be computed in $\mathcal{O}(M \log M + r \log(1/\varepsilon))$ operations (where ε is the required accuracy) using Beylkin’s unequally spaced FFT algorithm [4].

Step 2: We solve $T_M a_M = y_M$ by the conjugate gradient (CG) algorithm [18]. The matrix-vector multiplication in each iteration of CG can be carried out in $\mathcal{O}(M \log M)$ operations via FFT [8]. Thus the solution of (27) takes $\mathcal{O}(kM \log M)$ operations, where k is the number of iterations.

Step 3: Usually, the signal is reconstructed on regularly space nodes $\{u_i\}_{i=1}^N$. In this case $p_M(u_i)$ in (28) can be computed by FFT. For non-uniformly spaced nodes u_i we can again resort to Beylkin’s USFFT algorithm.

There exists a large number of fast algorithms for the solution of Toeplitz systems. Probably the most efficient algorithm in our case is CG. We have already mentioned that the Toeplitz system (27) can be solved in $\mathcal{O}(kM \log M)$ via CG. The number of iterations k depends essentially on the clustering of the eigenvalues of T_M , cf. [8]. It follows from equation (31) below and perturbation theory [10] that, if the sampling points stem from a perturbed regular sampling set, the eigenvalues of T_M will be clustered around β , where β is the oversampling rate. In such cases we can expect a very fast rate of convergence. The simple frame iteration [26,1] is not able to take advantage of such a situation.

For the analysis of the relation between the solution p_M of Theorem 3.1 and the solution f of the original infinite-dimensional problem we follow Gröchenig [20]. Assume that the samples $\{f(t_j)\}_{j \in \mathbb{Z}}$ of $f \in \mathbf{B}$ are given. For the finite-dimensional approximation we consider only those samples $f(t_j)$

for which t_j is contained in the interval $[-M - \frac{1}{2}, M + \frac{1}{2}]$ and compute the least-squares approximation p_M with degree M and period $2M + 1$ as in Theorem 3.1. It is shown in [20] that if $\sigma(T_M) \subseteq [\alpha, \beta]$ for all M with $\alpha > 0$ then

$$\lim_{M \rightarrow \infty} \int_{[-M, M]} |f(t) - p_M(t)|^2 dt = 0 \tag{29}$$

and also $\lim p_M(t) = f(t)$ uniformly on compact sets.

Under the Nyquist condition $\sup(t_{j+1} - t_j) := \gamma < 1$ and using weights $w_j = (t_{j+1} - t_{j-1})/2$ Gröchenig has shown that

$$\sigma(T_M) \subseteq [(1 - \gamma)^2, 6], \tag{30}$$

independently of M , see [20]. These results validate the usage of trigonometric polynomials as finite-dimensional model for nonuniform sampling.

Example 1 (Reconsidered). Recall that in Example 1 of Section 2 we have considered the reconstruction of a regularly oversampled signal $f \in \mathcal{B}$. What does the reconstruction method of Theorem 3.1 yield in this case? Let us check the entries of the matrix T_M when we take only those samples in the interval $[-n, n]$. The period of the polynomial becomes $2N$ with $N = n + \frac{n}{r-1}$ where r is the number of given samples. Then

$$(T_M)_{k,l} = \frac{1}{2N} \sum_{j=1}^r e^{2\pi i(k-l)t_j/(2N)} = \sum_{j=-nm}^{nm} e^{2\pi i(k-l)j/(2nm+1)} = m\delta_{k,l} \tag{31}$$

for $k, l = -M, \dots, M$, where $\delta_{k,l}$ is Kronecker’s symbol with the usual meaning $\delta_{k,l} = 1$ if $k = l$ and 0 else. Hence we get

$$T_M = mI,$$

where I is the identity matrix on \mathbb{C}^{2M+1} , thus T_M resembles the structure of the infinite-dimensional frame operator S in this case (including exact approximation of the frame bounds). Recall that the truncated frame approach leads to an “artificial” ill-posed problem even in such a simple situation.

The advantages of the trigonometric polynomial approach compared to the truncated frame approach are manifold. In the one case we have to deal with an ill-posed problem which has no specific structure, hence its solution is numerically very expensive. In the other case we have to solve a problem with rich mathematical structure, whose stability depends only on the sampling density, a situation that resembles the original infinite-dimensional sampling problem.

In principle, the coefficients $a_M = \{(a_M)_k\}_{k=-M}^M$ of the polynomial p_M that minimizes (24) could also be computed by directly solving the Vandermonde-type system

$$W V a_M = W b, \tag{32}$$

where $V_{j,k} = (1/\sqrt{2M+1})e^{-2\pi i k t_j/(2M+1)}$ for $j = 1, \dots, r, k = -M, \dots, M$ and W is a diagonal matrix with entries $W_{j,j} = \sqrt{w_j}$, cf. [31]. Several algorithms are known for a relatively efficient solution of Vandermonde systems [5,31]. However this is one of the rare cases, where, instead of directly solving (32), it is advisable to explicitly establish the system of normal equations

$$T_M a_M = y_M, \tag{33}$$

where $T = V^* W^2 V$ and $y = V^* W^2 b$.

The advantages of considering the system $T_M a_M = y_M$ instead of the Vandermonde system (32) are manifold:

- The matrix T_M plays a key role in the analysis of the relation of the solution of (24) and the solution of the infinite-dimensional sampling problem (9), see (29) and (30) above.
- T_M is of size $(2M + 1) \times (2M + 1)$, independently of the number of sampling points. Moreover, since $(T_M)_{k,l} = \sum_{j=1}^r w_j e^{2\pi i(k-l)t_j}$, it is of Toeplitz type. These facts give rise to fast and robust reconstruction algorithms.
- The resulting reconstruction algorithms can be easily generalized to higher dimensions, see Section 3.1. Such a generalization to higher dimensions seems not to be straightforward for fast solvers of Vandermonde systems such as the algorithm proposed in [31].

We point out that other finite-dimensional approaches are proposed in [16,7]. These approaches may provide interesting alternatives in the few cases where the algorithm outlined in Section 3 does not lead to good results. These cases occur when only a few samples of the signal f are given in an interval $[a, b]$ say, and at the same time we have $|f(a) - f(b)| \gg 0$ and $|f'(a) - f'(b)| \gg 0$, i.e., if f is “strongly nonperiodic” on $[a, b]$. However the computational complexity of the methods in [16,7] is significantly larger.

3.1. Multi-dimensional nonuniform sampling

The approach presented above can be easily generalized to higher dimensions by a diligent book-keeping of the notation. We consider the space of d -dimensional trigonometric polynomials \mathbf{P}_M^d as finite-dimensional model for \mathbf{B}^d . For given samples $f(t_j)$ of $f \in \mathbf{B}^d$, where $t_j \in \mathbb{R}^d$, we compute the least-squares approximation p_M similar to Theorem 3.1 by solving the corresponding system of equations $T_M a_M = y_M$.

In 2-D for instance the matrix T_M becomes a block Toeplitz matrix with Toeplitz blocks [37]. For a fast computation of the entries of T we can again make use of Beylkin’s USFFT algorithm [4]. And similar to 1-D, multiplication of a vector by T_M can be carried out by 2-D FFT.

Also the relation between the finite-dimensional approximation in \mathbf{P}_M^d and the infinite-dimensional solution in \mathbf{B}^d is similar as in 1-D. The only mathematical difficulty is to give conditions under which the matrix T_M is invertible. Since the fundamental theorem of algebra does not hold in dimensions larger than one, the condition $(2M + 1)^d \leq r$ is necessary but no longer sufficient for the invertibility of T_M . Sufficient conditions for the invertibility, depending on the sampling density, are presented in [21].

4. Bandwidth estimation and regularization

In this section we discuss several numerical aspects of nonuniform sampling that are very important from a practical viewpoint, however only few answers to these problems can be found in the literature.

4.1. A multilevel signal reconstruction algorithm

In almost all theoretical results and numerical algorithms for reconstructing a band-limited signal from nonuniform samples it is assumed that the bandwidth is known a priori. This information however is often not available in practice.

A good choice of the bandwidth for the reconstruction algorithm becomes crucial in case of noisy data. It is intuitively clear that choosing a too large bandwidth leads to over-fit of the noise in the data, while a too small bandwidth yields a smooth solution but also to under-fit of the data. And of course we want to avoid the determination of the “correct” Ω by trial-and-error methods. Hence the problem is to design a method that can reconstruct a signal from nonuniformly spaced, noisy samples without requiring a priori information about the bandwidth of the signal.

The multilevel approach derived in [34] provides an answer to this problem. The approach applies to an infinite-dimensional as well as to a finite-dimensional setting. We describe the method directly for the trigonometric polynomial model, where the determination of the bandwidth Ω translates into the determination of the polynomial degree M of the reconstruction. The idea of the multilevel algorithm is as follows.

Let the noisy samples $\{b_j^\delta\}_{j=1}^r = \{f^\delta(t_j)\}_{j=1}^r$ of $f \in \mathbf{B}$ be given with $\sum_{j=1}^r |f(t_j) - b_j^\delta|^2 \leq \delta^2 \|b^\delta\|^2$ and let Q_M denote the orthogonal projection from \mathbf{B} into \mathbf{P}_M . We start with initial degree $M = 1$ and run Algorithm 3.1 until the iterates $p_{0,k}$ satisfy for the first time the *inner* stopping criterion

$$\sum_{j=1}^r |p_{1,k}(t_j) - b_j^\delta|^2 \leq 2\tau(\delta \|b^\delta\| + \|Q_0 f - f\|) \|b^\delta\|$$

for some fixed $\tau > 1$. Denote this approximation (at iteration k_*) by p_{1,k_*} . If p_{1,k_*} satisfies the *outer* stopping criterion

$$\sum_{j=1}^r |p_{1,k}(t_j) - b_j^\delta|^2 \leq 2\tau\delta \|b^\delta\|^2, \tag{34}$$

we take p_{1,k_*} as final approximation. Otherwise we proceed to the next level $M=2$ and run Algorithm 3.1 again, using p_{1,k_*} as initial approximation by setting $p_{2,0} = p_{1,k_*}$.

At level $M = N$ the inner level-dependent stopping criterion becomes

$$\sum_{j=1}^r |p_{N,k}(t_j) - b_j^\delta|^2 \leq 2\tau(\delta \|b^\delta\| + \|Q_N f - f\|) \|b^\delta\|, \tag{35}$$

while the outer stopping criterion does not change since it is level-independent.

Stopping rule (35) guarantees that the iterates of CG do not diverge. It also ensures that CG does not iterate too long at a certain level, since if M is too small further iterations at this level will not lead to a significant improvement. Therefore, we switch to the next level. The outer stopping criterion (34) controls over-fit and under-fit of the data, since in presence of noisy data it does not make sense to ask for a solution p_M that satisfies $\sum_{j=1}^r |p_M(t_j) - b_j^\delta|^2 = 0$.

Since the original signal f is not known, the expression $\|f - Q_N f\|$ in (35) cannot be computed. In [34] the reader can find an approach to estimate $\|f - Q_N f\|$ recursively.

4.2. *Solution of ill-conditioned sampling problems*

A variety of conditions on the sampling points $\{t_j\}_{j \in \mathbb{Z}}$ are known under which the set $\{\text{sinc}(\cdot - t_j)\}_{j \in \mathbb{Z}}$ is a frame for \mathbf{B} , which in turn implies (at least theoretically) perfect reconstruction of a signal f from its samples $f(t_j)$. This does however not guarantee a stable reconstruction from a numerical viewpoint, since the ratio of the frame bounds B/A can still be extremely large and therefore the frame operator S can be ill-conditioned. This may happen for instance if γ in (30) goes to 1, in which case $\text{cond}(T)$ may become large. The sampling problem may also become numerically unstable or even ill-posed, if the sampling set has large gaps, which is very common in astronomy and geophysics. Note that in this case the instability of the system $T_M a_M = y_M$ does *not* result from an inadequate discretization of the infinite-dimensional problem.

There exists a large number of (circulant) Toeplitz preconditioners that could be applied to the system $T_M a_M = y_M$, however it turns out that they do not improve the stability of the problem in this case. The reason lies in the distribution of the eigenvalues of T_M , as we will see below.

Following [38], we call two sequences of real numbers $\{\lambda_k^{(n)}\}_{k=1}^n$ and $\{v_k^{(n)}\}_{k=1}^n$ *equally distributed*, if

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n [F(\lambda_k^{(n)}) - F(v_k^{(n)})] = 0 \tag{36}$$

for any continuous function F with compact support.¹

Let C be an $(n \times n)$ circulant matrix with first column (c_0, \dots, c_{n-1}) , we write $C = \text{circ}(c_0, \dots, c_{n-1})$. The eigenvalues of C are distributed as $\lambda_k = (1/\sqrt{n}) \sum_{l=0}^{n-1} c_l e^{2\pi i k l / n}$. Observe that the Toeplitz matrix A_n with first column (a_0, a_1, \dots, a_n) can be embedded in the circulant matrix

$$C_n = \text{circ}(a_0, a_1, \dots, a_n, \bar{a}_n, \dots, \bar{a}_1). \tag{37}$$

Theorems 4.1 and 4.2 in [38] state that the eigenvalues of A_n and C_n are equally distributed as $f(x)$ where

$$f(x) = \sum_{k=-\infty}^{\infty} a_k e^{2\pi i k x}. \tag{38}$$

The partial sum of the series (38) is

$$f_n(x) = \sum_{k=-n}^n a_k e^{2\pi i k x}. \tag{39}$$

To understand the clustering behavior of the eigenvalues of T_M in case of sampling sets with large gaps, we consider a sampling set in $[-M, M)$, that consists of one large block of samples and one large gap, i.e., $t_j = j/Lm$ for $j = -mM, \dots, mM$, for $m, L \in \mathbb{N}$. (Recall that we identify the interval with the torus). Then the entries z_k of the Toeplitz matrix T_M of (28) (with $w_j = 1$) are

$$z_k = \frac{1}{2M + 1} \sum_{j=-mM}^{mM} e^{-2\pi i k j / Lm / (2M+1)}, \quad k = 0, \dots, 2M.$$

¹ In H. Weyl's definition $\lambda_k^{(n)}$ and $v_k^{(n)}$ are required to belong to a common interval.

To investigate the clustering behavior of the eigenvalues of T_M for $M \rightarrow \infty$, we embed T_M in a circulant matrix C_M as in (37). Then (39) becomes

$$f_{mM}(x) = \frac{1}{Lm(2M + 1)} \sum_{l=-mM}^{mM} \sum_{j=-mM}^{mM} e^{2\pi i l [k/(4M+1) - j/((2M+1)mL)]} \tag{40}$$

whence $f_{mM} \rightarrow \mathbf{1}_{[-1/(2L), 1/(2L)]}$ for $M \rightarrow \infty$, where $\mathbf{1}_{[-a, a]}(x) = 1$, if $-a < x < a$ and 0 else.

Thus the eigenvalues of T_M are asymptotically clustered around zero and one. For general nonuniform sampling sets with large gaps the clustering at 1 will disappear, but of course the spectral cluster at 0 will remain. In this case it is known that the preconditioned problem will still have a spectral cluster at the origin [43] and preconditioning will not be efficient.

Fortunately, there are other possibilities to obtain a stabilized solution of $T_M a_M = y_M$. The condition number of T_M essentially depends on the ratio of the maximal gap in the sampling set to the Nyquist rate, which in turn depends on the bandwidth of the signal. We can improve the stability of the system by adapting the degree M of the approximation accordingly. Thus the parameter M serves as a regularization parameter that balances stability and accuracy of the solution. This technique can be seen as a specific realization of *regularization by projection*, see [12, Chapter 3]. In addition, as described in Section 4.2, we can utilize CG as regularization method for the solution of the Toeplitz system in order to balance approximation error and propagated error. The multilevel method introduced in Section 4.1 combines both features. By optimizing the level (bandwidth) and the number of iterations in each level it provides an efficient and robust regularization technique for ill-conditioned sampling problems. See Section 5 for numerical examples.

5. Applications

We present two numerical examples to demonstrate the performance of the described methods. The first one concerns a 1-D reconstruction problem arising in spectroscopy. In the second example we approximate the Earth’s magnetic field from noisy scattered data.

5.1. An example from spectroscopy

The original spectroscopy signal f is known at 1024 regularly spaced points t_j . This discrete sampling sequence will play the role of the original continuous signal. To simulate the situation of a typical experiment in spectroscopy we consider only 107 randomly chosen sampling values of the given sampling set. Furthermore, we add noise to the samples with noise level (normalized by division by $\sum_{k=1}^{1024} |f(t_k)|^2$) of $\delta = 0.1$. Since the samples are contaminated by noise, we cannot expect to recover the (discrete) signal f completely. The bandwidth is approximately $\Omega = 5$ which translates into a polynomial degree of $M \approx 30$. Note that in general Ω and (hence M) may not be available. We will also consider this situation, but in the first experiments we assume that we know Ω . The error between the original signal f and an approximation f_n is measured by computing $\|f - f_n\|^2 / \|f\|^2$.

First we apply the truncated frame method with regularized SVD as described in Section 2. We choose the truncation level for the SVD via formula (21). This is the optimal truncation level in this case, providing an approximation with least-squares error 0.0944. Fig. 1(a) shows the reconstructed

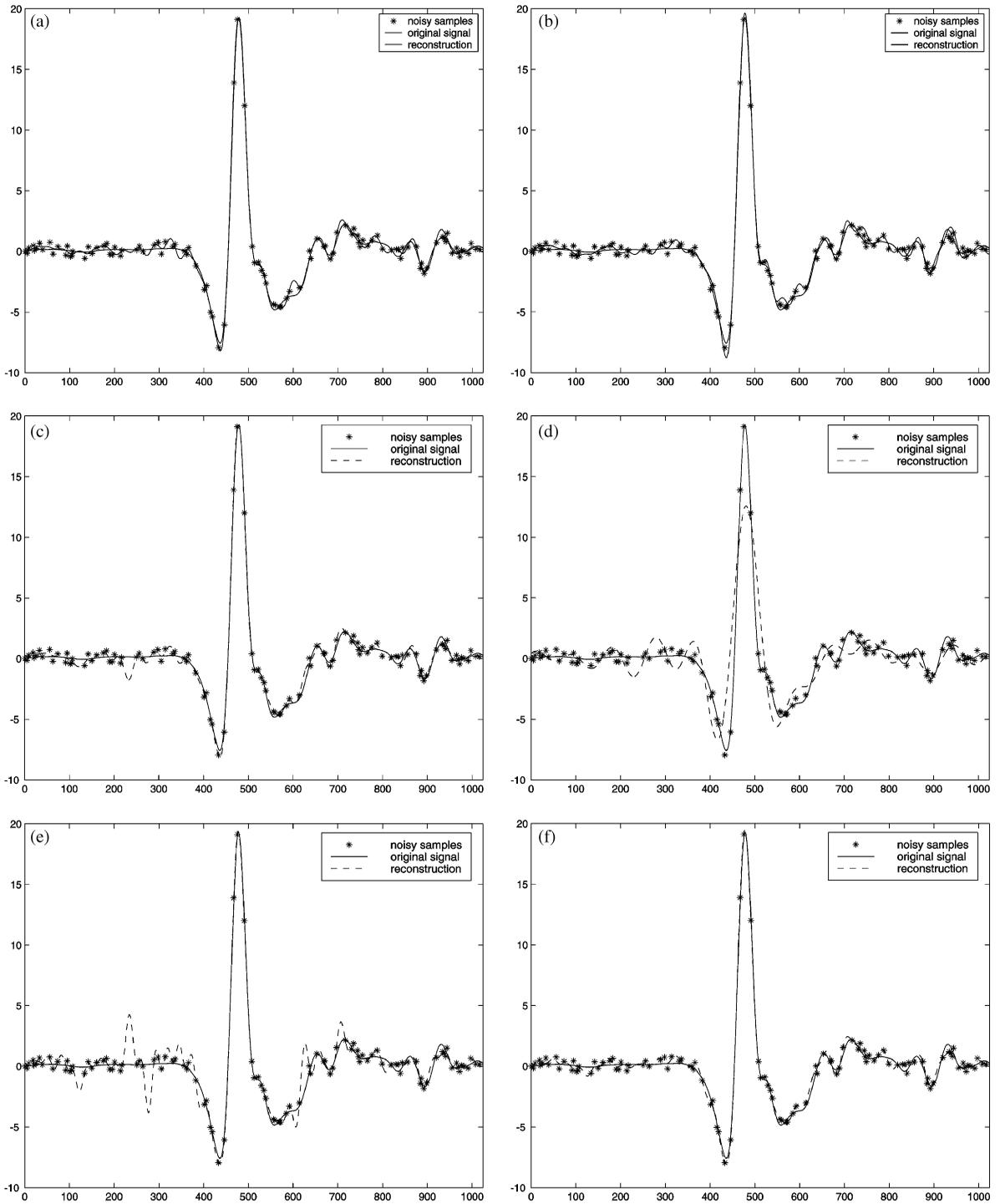


Fig. 1. Example from spectroscopy-comparison of reconstruction methods. (a) Truncated frame method with TSVD, error=0.0944. (b) Truncated frame method with CG, error=0.1097. (c) Algorithm 3.1 with "correct" bandwidth, error=0.0876. (d) Using a too small bandwidth, error=0.4645. (e) Using a too large bandwidth, error=0.2412. (f) Multilevel algorithm, error=0.0959.

signal together with the original signal and the noisy samples. Without regularization we get a much worse “reconstruction” (which is not displayed).

We apply CG to the truncated frame method, as proposed in Section 2.2 with stopping criterion (22) (for $\tau = 1$). The algorithm terminates already after 3 iterations. The reconstruction error is with 0.1097 slightly higher than for truncated SVD (see also Fig. 1(b)), but the computational effort is much smaller.

Also Algorithm 3.1 (with $M = 30$) terminates after 3 iterations. The reconstruction is shown in Fig. 1(c), the least squares error (0.0876) is slightly smaller than for the truncated frame method, the computational effort is significantly smaller.

We also simulate the situation where the bandwidth is not known a priori and demonstrate the importance of a good estimate of the bandwidth. We apply Algorithm 3.1 using a too small degree ($M = 11$) and a too high degree ($M = 40$). (We get qualitatively the same results using the truncated frame method when using a too small or too large bandwidth.) The approximations are shown in Figs. 1(d) and (e). The approximation errors are 0.4648 and 0.2805, respectively. Now we apply the multilevel algorithm of Section 4.1 which does not require any initial choice of the degree M . The algorithm terminates at “level” $M = 22$, the approximation is displayed in Fig. 1(f), the error is 0.0959, thus within the error bound δ , as desired. Hence without requiring explicit information about the bandwidth, we are able to obtain the same accuracy as for the methods above.

5.2. Approximation of geophysical potential fields

Exploration geophysics relies on surveys of the Earth’s magnetic field for the detection of anomalies which reveal underlying geological features. Geophysical potential field data are generally observed at scattered sampling points. Geoscientists, used to looking at their measurements on maps or profiles and aiming at further processing, therefore need a representation of the originally irregularly spaced data at a regular grid.

The reconstruction of a 2-D signal from its scattered data is thus one of the first and crucial steps in geophysical data analysis, and a number of practical constraints such as measurement errors and the huge amount of data make the development of reliable reconstruction methods a difficult task.

It is known that the Fourier transform of a geophysical potential field f has decay $|\hat{f}(\omega)| = \mathcal{O}(e^{-|\omega|})$. This rapid decay implies that f can be very well approximated by band-limited functions [30]. Since, in general, we may not know the (essential) bandwidth of f , we can use the multilevel algorithm proposed in Section 4.1 to reconstruct f .

The multilevel algorithm also takes care of following problem. Geophysical sampling sets are often highly anisotropic and large gaps in the sampling geometry are very common. The large gaps in the sampling set can make the reconstruction problem ill-conditioned or even ill-posed. As outlined in Section 4.2 the multilevel algorithm iteratively determines the optimal bandwidth that balances the stability and accuracy of the solution.

Fig. 2(a) shows a synthetic gravitational anomaly f . The spectrum of f decays exponentially, thus the anomaly can be well represented by a band-limited function, using a “cut-off-level” of $|f(\omega)| \leq 0.01$ for the essential bandwidth of f .

We have sampled the signal at 1000 points (u_j, v_j) and added 5% random noise to the sampling values $f(u_j, v_j)$. The sampling geometry – shown in Fig. 2 as black dots – exhibits several features one encounters frequently in exploration geophysics [30]. The essential bandwidth of f would imply

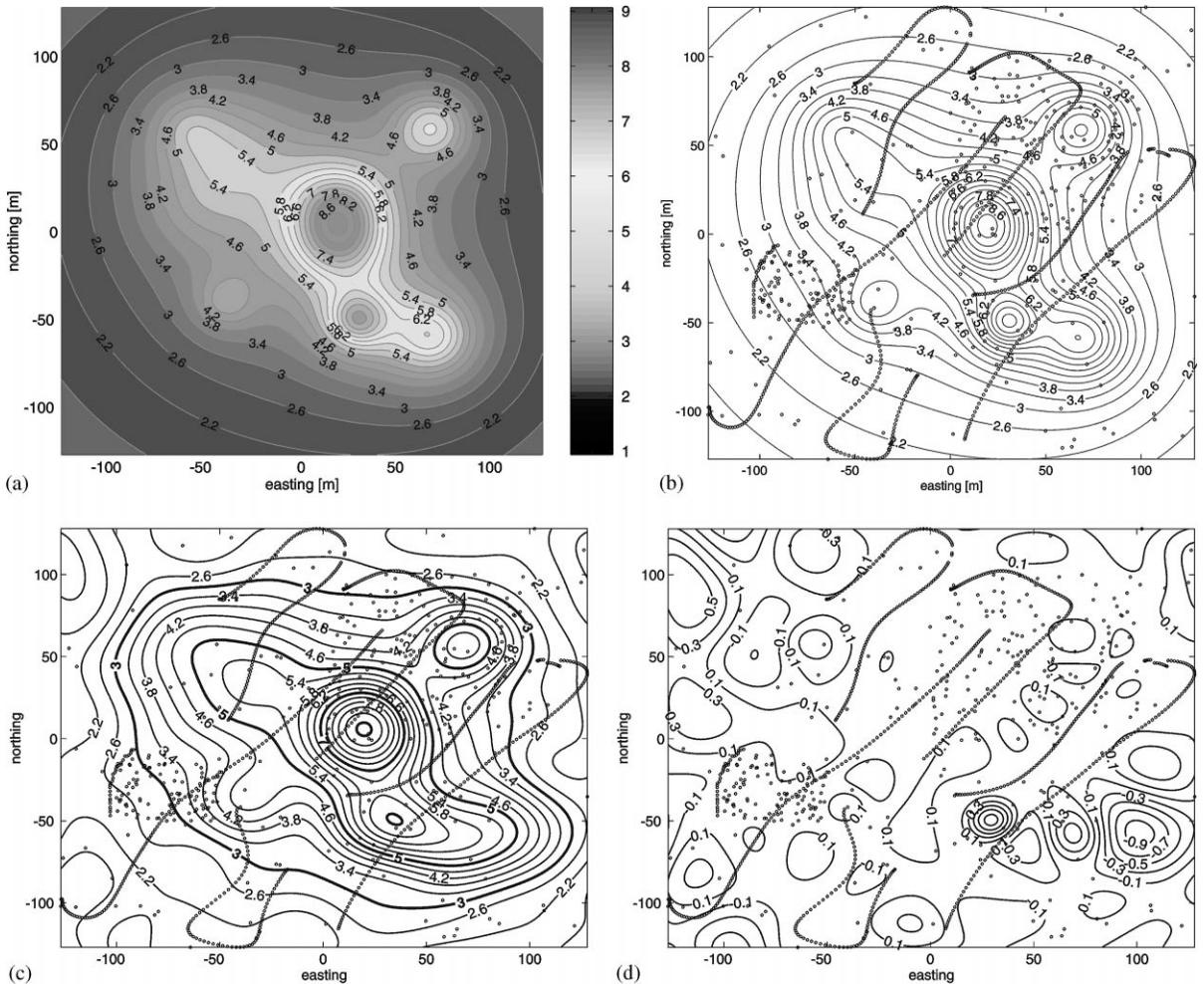


Fig. 2. Approximation of synthetic gravity anomaly from 1000 nonuniformly spaced noisy samples by the multilevel algorithm of Section 4.1. The algorithm iteratively determines the optimal bandwidth (i.e. level) for the approximation. (a) Contour map of synthetic gravity anomaly, gravity is in mGal. (b) Sampling set and synthetic gravity anomaly. (c) Approximation by multi-level algorithm. (d) Error between approximation and actual anomaly.

to choose a polynomial degree of $M = 12$ (i.e., $(2M + 1)^2 = 625$ spectral coefficients). With this choice of M the corresponding block Toeplitz matrix T_M would become ill-conditioned, making the reconstruction problem unstable. As mentioned above, in practice we usually do not know the essential bandwidth of f . Hence we will not make use of this knowledge in order to approximate f .

We apply the multilevel method to reconstruct the signal, using only the sampling points $\{(u_j, v_j)\}$, the samples $\{f^\delta(u_j, v_j)\}$ and the noise level $\delta=0.05$ as a priori information. The algorithm terminates at level $M = 7$. The reconstruction is displayed in Fig. 2(c), the error between the true signal and the approximation is shown in Fig. 2(d). The reconstruction error is 0.0517 (or 0.193 mGal), thus of the same order as the data error, as desired.

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Asymptotic expansions for multivariate polynomial approximation

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Abstract

In this paper the approximation of multivariate functions by (multivariate) Bernstein polynomials is considered. Building on recent work of Lai (J. Approx. Theory 70 (1992) 229–242), we can prove that the sequence of these Bernstein polynomials possesses an asymptotic expansion with respect to the index n . This generalizes a corresponding result due to Costabile et al. (BIT 36 (1996) 676–687) on univariate Bernstein polynomials, providing at the same time a new proof for it. After having shown the existence of an asymptotic expansion we can apply an extrapolation algorithm which accelerates the convergence of the Bernstein polynomials considerably; this leads to a new and very efficient method for polynomial approximation of multivariate functions. Numerical examples illustrate our approach. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Asymptotic expansion; Bernstein operator; Convergence acceleration; Extrapolation; Multivariate polynomial approximation

1. Introduction and preliminaries

One of the fundamental questions in extrapolation theory is the following one: Can the convergence of a given sequence be accelerated by a suitable extrapolation algorithm or not? The oldest and up to the present day most widespread criterion for a positive answer to this question is the existence of an asymptotic expansion for the sequence to be accelerated (see the next section for exact definitions).

This is the reason why the terms asymptotic expansion and extrapolation are so deeply connected. Now, the next question is: Where in Applied Analysis do exist sequences with this property? It is the main reason of this paper, which is both a survey and a research paper, to convince the reader that this is the case also in a field where this was not so well-known until now: Approximation of multivariate functions by polynomials.

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We first shortly review what kind of asymptotic expansion we are looking at, and what the corresponding extrapolation process looks like. For more details on these topics, see [7].

Definition. Let there be given a sequence of real or complex numbers $\{\sigma_n\}$ and natural numbers m and N . The sequence $\{\sigma_n\}$ is said to possess an asymptotic expansion of order m , if each σ_n for $n > N$ can be written in the form

$$\sigma_n = \sum_{\mu=0}^m \frac{c_\mu}{n^{\rho_\mu}} + o(n^{-\operatorname{Re} \rho_m}) = c_0 + \sum_{\mu=1}^m \frac{c_\mu}{n^{\rho_\mu}} + o(n^{-\operatorname{Re} \rho_m}) \quad \text{for } n \rightarrow \infty. \tag{1}$$

Here, the exponents $\{\rho_\mu\}$ are real or complex numbers with the property

$$\rho_0 = 0 \quad \text{and} \quad \operatorname{Re} \rho_\mu < \operatorname{Re} \rho_{\mu+1} \quad \text{for all } \mu \in \mathbb{N}_0.$$

Moreover, if a sequence $\{\sigma_n\}$ possesses an expansion of type (1) for all $m \in \mathbb{N}$, then we say that the expansion is of arbitrary order, and write

$$\sigma_n = c_0 + \sum_{\mu=1}^{\infty} \frac{c_\mu}{n^{\rho_\mu}} \tag{2}$$

for short.

Asymptotic expansions of the type (1) are sometimes also denoted in more detail as logarithmic asymptotic expansions (see [5] or [7]). In this paper, we will use the abbreviated notation asymptotic expansion only.

It is well known (cf., e.g., [1,7]) that the basic idea of extrapolation applied to such sequences is to compute the values of σ_n for several choices of n , say $n = n_0 < n_1 < n_2 < \dots$, and to combine them in order to obtain new sequences, which converge faster than the original ones. For many applications it is convenient to choose the sequence $\{n_i\}$ not just anyhow, but as a geometric progression: With natural numbers n_0 and b , $b \geq 2$, we put

$$n_i := n_0 b^i, \quad i = 0, 1, 2, \dots \tag{3}$$

Then the extrapolation process reads as follows (cf. (4)):

Lemma 1. *Let there be given a sequence $\{\sigma_n\}$, which possesses an asymptotic expansion of the form (1), and a sequence of natural numbers $\{n_i\}$, satisfying (3). Furthermore, choose some $K \in \mathbb{N}$, $K \leq m$ and define for $k = 0, \dots, K$ new sequences $\{y_i^{(k)}\}_{i \in \mathbb{N}}$ through the process*

$$\begin{aligned} y_i^{(0)} &= \sigma_{n_i}, \quad i = 0, 1, \dots, \\ y_i^{(k)} &= \frac{b^{\rho_k} \cdot y_{i+1}^{(k-1)} - y_i^{(k-1)}}{b^{\rho_k} - 1} \quad \begin{cases} k = 1, 2, \dots, K, \\ i = 0, 1, \dots \end{cases} \end{aligned} \tag{4}$$

Then each of the sequences $\{y_i^{(k)}\}_{i \in \mathbb{N}}$ possesses an asymptotic expansion of the form

$$y_i^{(k)} = c_0 + \sum_{\mu=k+1}^m \frac{c_\mu^{(k)}}{n_i^{\rho_\mu}} + o(n_i^{-\operatorname{Re} \rho_m}) \quad \text{for } n_i \rightarrow \infty \tag{5}$$

with coefficients $c_\mu^{(k)}$ independent of n_i . In particular, each of the sequences $\{y_i^{(k)}\}$ converges faster to the limit c_0 than its predecessor.

So, the message is: If one has a convergent numerical process of whatever kind, say, a discretized differential equation or a quadrature formula, one should always check whether the output of this process has an asymptotic expansion. Experience says that this is indeed the case in much more situations than commonly expected or known.

To illustrate and to support this remark, we consider in this paper the Bernstein polynomial operators (or Bernstein polynomials), which are in Approximation Theory well known as a tool for polynomial approximation of functions. It will be shown that the sequence of these operators also possesses an asymptotic expansion, and thus that their order of convergence can be improved considerably using extrapolation. In the univariate case, this result was proved quite recently in [2] (see Theorem 2). As the main new contribution, we develop an analogous result for the multivariate case. Since the proof in [2] cannot be adopted for the multivariate case, we had to develop a new approach, building on results published in [3]. This provides at the same time a new proof also for the univariate case.

2. Asymptotic expansion for the Bernstein operator

We first briefly review some results on the univariate case and then prove our main result (Theorem 5) on the multivariate one.

The sequence of Bernstein operators

$$B_n(f; x) := \sum_{v=0}^n f\left(\frac{v}{n}\right) B_{n,v}(x), \quad (6)$$

defined for any $f \in C[0, 1]$, converges uniformly to f on $[0, 1]$. Here, $B_{n,v}(x)$ denotes the (univariate) Bernstein polynomial

$$B_{n,v}(x) := \binom{n}{v} x^v (1-x)^{n-v}.$$

However, as shown by Voronovskaja [6], we have

$$\lim_{n \rightarrow \infty} n(B_n(f; x) - f(x)) = \frac{x(1-x)}{2} f^{(2)}(x) \quad (7)$$

in each point $x \in [0, 1]$ where $f^{(2)}(x)$ exists.

This means that already quadratic polynomials are not reproduced by $B_n(f; \cdot)$, and that the order of convergence is not better than $O(1/n)$. Therefore, several attempts have been made to improve this order of convergence, see [2] for an overview and some references.

In view of asymptotic expansion and extrapolation theory, a big step was done recently in [2], who established the asymptotic expansion for the Bernstein operator B_n . Their main result can be stated as follows:

Theorem 2. *Let $f \in C^{2k}[0, 1]$ with some $k \in \mathbb{N}$. Then the sequence $\{B_n(f; x)\}$, defined in (6), possesses an asymptotic expansion of the form*

$$B_n(f; x) = f(x) + \sum_{v=1}^k \frac{c_v(x)}{n^v} + o(n^{-k}) \quad \text{for } n \rightarrow \infty.$$

It is our goal to develop an analogous result for the multivariate case.

However, we do *not* generalize the proof given in [2], which could by the way be shortened considerably by using the asymptotic results already to be found in [4]. Instead, we will make use of some asymptotic relations for multivariate Bernstein polynomials, established quite recently in [3].

Let v^0, \dots, v^s be $(s + 1)$ distinct points in \mathbb{R}^s , such that the volume of the s -simplex $T := \langle v^0, \dots, v^s \rangle$ is positive. For each point $\mathbf{x} \in T$, we denote by $(\lambda_0, \dots, \lambda_s)$ the barycentric coordinates of \mathbf{x} w.r.t. T .

It is well known that any polynomial $p_n(\mathbf{x})$ of total degree n can be expressed by using the basic functions

$$B_\alpha(\lambda) := \frac{|\alpha|!}{\alpha!} \lambda^\alpha, \quad \alpha \in \mathbb{N}_0^{s+1} \quad \text{with } |\alpha| = n$$

in the form

$$p_n(\mathbf{x}) = \sum_{\substack{|\alpha|=n \\ \alpha \in \mathbb{N}_0^{s+1}}} c_\alpha B_\alpha(\lambda), \quad \mathbf{x} \in T.$$

Here, as usual, for any $\alpha = (\alpha_0, \dots, \alpha_s) \in \mathbb{N}_0^{s+1}$, we set $|\alpha| = \alpha_0 + \dots + \alpha_s$ and $\alpha! = \alpha_0! \cdots \alpha_s!$. Also, it is $\lambda^\alpha = \lambda_0^{\alpha_0} \cdots \lambda_s^{\alpha_s}$.

For each $\alpha \in \mathbb{N}_0^{s+1}$, denote by \mathbf{x}_α the point

$$\mathbf{x}_\alpha := \frac{1}{|\alpha|} \sum_{i=0}^s \alpha_i v^i.$$

We consider the approximation of a given function $f \in C(T)$ by the multivariate Bernstein polynomial

$$B_n(f; \mathbf{x}) := \sum_{\substack{|\alpha|=n \\ \alpha \in \mathbb{N}_0^{s+1}}} f(\mathbf{x}_\alpha) B_\alpha(\lambda). \tag{8}$$

As in [3], we introduce the auxiliary polynomials

$$S_\gamma^n(\mathbf{x}) = n^{|\gamma|} \sum_{\substack{|\alpha|=n \\ \alpha \in \mathbb{N}_0^{s+1}}} (\mathbf{x}_\alpha - \mathbf{x})^\gamma B_\alpha(\lambda)$$

for $\gamma \in \mathbb{N}_0^s$. The following results, which we will make use of below, were proved in [3].

Theorem 3. *The polynomials S_γ^n possess the explicit representations*

$$S_\gamma^n \equiv 0 \quad \text{for } |\gamma| \leq 1,$$

$$S_\gamma^n(\mathbf{x}) = n \sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^\gamma \quad \text{for } |\gamma| = 2,$$

and

$$S_\gamma^n(\mathbf{x}) = \sum_{\mu=1}^{|\gamma|-2} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} n(n-1) \cdots (n-\mu+1) \prod_{i=1}^\mu \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) \quad \text{for } |\gamma| \geq 3.$$

Theorem 4. For $k \in \mathbb{N}$ and $f \in C^{2k}(T)$, we have

$$\lim_{n \rightarrow \infty} n^k \left[B_n(f; \mathbf{x}) - f(\mathbf{x}) - \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma| \leq 2k-1}} \frac{1}{\gamma!} \frac{S_\gamma^n(\mathbf{x})}{n^{|\gamma|}} D^\gamma f(\mathbf{x}) \right] = \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2k}} \frac{1}{\gamma!} \sum_{\substack{\beta^1, \dots, \beta^k \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^k = \gamma \\ |\beta^i| \geq 2, i=1, \dots, k}} \prod_{i=1}^k \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) D^\gamma f(\mathbf{x}). \tag{9}$$

Building on these auxiliary results, we can now state and prove our main theorem. Note that although Theorem 4 is a deep and nice result on the asymptotic behavior of the multivariate Bernstein approximants, it does still not yet prove the asymptotic expansion. To do this, a careful analysis of the coefficient functions in (9) is necessary.

Theorem 5. Let $f \in C^{2k}(T)$ with some $k \in \mathbb{N}$. Then the sequence of Bernstein approximants $\{B_n(f; \mathbf{x})\}$, defined in (8), possesses an asymptotic expansion of the form

$$B_n(f; \mathbf{x}) = f(\mathbf{x}) + \sum_{v=1}^k \frac{c_v(\mathbf{x})}{n^v} + o(n^{-k}) \quad \text{for } n \rightarrow \infty. \tag{10}$$

The coefficient functions $c_v(\mathbf{x})$ can be given explicitly; we have

$$c_v(\mathbf{x}) = \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ v+1 \leq |\gamma| \leq 2v}} \frac{1}{\gamma!} \sum_{\mu=|\gamma|-v}^{\lfloor |\gamma|/2 \rfloor} \alpha_{|\gamma|-v, \mu} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^\mu \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) \tag{11}$$

with recursively computable numbers $\alpha_{i, \mu}$, see (14) below.

Proof. We use the following result, to be found for example in [7].

A sequence $\{B_n\}$ possesses an asymptotic expansion of the desired form, if and only if for $m = 1, \dots, k$,

$$\lim_{n \rightarrow \infty} n^m \left\{ B_n - f - \sum_{v=1}^{m-1} \frac{c_v}{n^v} \right\} = : c_m \tag{12}$$

exists and is different from zero. (Here and below, we set empty sums equal to zero.)

From (12), it is clear that the results due to Lai, as quoted above, are a big step towards the proof of our Theorem, but as be seen below, there is still something to do.

We first have to make a further analysis of the functions S_γ^n . It is clear that if we have points $\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s$ with $|\beta^i| \geq 2, i = 1, \dots, \mu$, and if $\mu > |\gamma|/2$, then

$$|\beta^1 + \dots + \beta^\mu| > |\gamma|.$$

This means that

$$\begin{aligned} \frac{S_\gamma^n(\mathbf{x})}{n^{|\gamma|}} &= \sum_{\mu=1}^{|\gamma|-2} \frac{n(n-1)\cdots(n-\mu+1)}{n^{|\gamma|}} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) \\ &= \sum_{\mu=1}^{\lfloor |\gamma|/2 \rfloor} \frac{n(n-1)\cdots(n-\mu+1)}{n^{|\gamma|}} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) \end{aligned} \tag{13}$$

with

$$\left\lfloor \frac{|\gamma|}{2} \right\rfloor = \begin{cases} \frac{|\gamma|}{2}, & |\gamma| \text{ even,} \\ \frac{|\gamma|-1}{2}, & |\gamma| \text{ odd.} \end{cases}$$

Next, we observe that the expression

$$n(n-1)\cdots(n-\mu+1)$$

is a polynomial of exact degree μ in n , say

$$n(n-1)\cdots(n-\mu+1) = \sum_{i=1}^{\mu} \alpha_{i,\mu} n^i,$$

with coefficients $\alpha_{i,\mu}$, which can be computed by the recursion

$$\alpha_{1,1} = 1, \quad \alpha_{i,1} = 0, \quad i \neq 1,$$

and

$$\alpha_{i,\mu+1} := \alpha_{i-1,\mu} - \mu \alpha_{i,\mu}, \quad \mu \geq 1, \quad 1 \leq i \leq \mu + 1. \tag{14}$$

In particular,

$$\alpha_{\mu,\mu} = 1 \quad \text{and} \quad \alpha_{1,\mu} = (-1)^{\mu-1} (\mu - 1)! \tag{15}$$

for all μ .

Together with (13), it follows that

$$\frac{S_\gamma^n(\mathbf{x})}{n^{|\gamma|}} = \sum_{\mu=1}^{\lfloor |\gamma|/2 \rfloor} \sum_{i=1}^{\mu} \frac{\alpha_{i,\mu}}{n^{|\gamma|-i}} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right). \tag{16}$$

Rearranging this according to powers of n , we obtain

$$\frac{S_\gamma^n(\mathbf{x})}{n^{|\gamma|}} = \sum_{l=\lfloor |\gamma|+1/2 \rfloor}^{|\gamma|-1} \frac{\delta_{l,\gamma}(\mathbf{x})}{n^l} \tag{17}$$

with coefficient functions $\delta_{l,\gamma}$, which do not depend on n .

For later use, we note that for $|\gamma|$ even, say $|\gamma| = 2v$, the coefficient of the lowest power of n , $\delta_{v,\gamma}$, can be given explicitly: From (16), we deduce that

$$\begin{aligned} \delta_{v,\gamma}(\mathbf{x}) &= \alpha_{v,\gamma} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) \\ &= \sum_{\substack{\beta^1, \dots, \beta^v \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^v = 2v \\ |\beta^i| = 2, i=1, \dots, v}} \prod_{i=1}^v \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right). \end{aligned} \tag{18}$$

From (17), it follows that the sum over all these expressions itself is of the form

$$\sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma| \leq 2k-1}} \frac{1}{\gamma!} \frac{S_\gamma^n(\mathbf{x})}{n^{|\gamma|}} D^\gamma f(\mathbf{x}) = \frac{d_{1,k}(\mathbf{x})}{n} + \frac{d_{2,k}(\mathbf{x})}{n^2} + \dots + \frac{d_{k,k}(\mathbf{x})}{n^k} + O(n^{-(k+1)}). \tag{19}$$

We now make the

Claim. For all $v \leq k$, the coefficient functions $d_{j,v}$ in (19) satisfy

$$d_{j,v}(\mathbf{x}) = d_{j,v-1}(\mathbf{x}) \quad j = 1, \dots, v - 2$$

and

$$d_{v-1,v}(\mathbf{x}) = d_{v-1,v-1}(\mathbf{x}) + \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2v-2}} \delta_{v-1,\gamma}(\mathbf{x}) \tag{20}$$

with $\delta_{v-1,2v-1}$ from (17).

Proof of Claim. The proof is by induction. For $k = 1$, there is nothing to show, while for $k = 2$, the only relation to prove is

$$d_{1,2}(\mathbf{x}) = d_{1,1}(\mathbf{x}) + \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2}} \delta_{1,\gamma}(\mathbf{x}).$$

But this is true, since $d_{1,1} = 0$.

Now we assume that the claim is true for v , and prove it for $v + 1$.

From (17) and (19) and the induction hypothesis,

$$\sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma| \leq 2v+1}} \frac{1}{\gamma!} \frac{S_\gamma^n}{n^{|\gamma|}} D^\gamma f(\mathbf{x})$$

$$\begin{aligned}
 &= \frac{d_{1,v}(\mathbf{x})}{n} + \dots + \frac{d_{v,v}(\mathbf{x})}{n^v} + O(n^{-(v+1)}) + \sum_{l=v}^{2v-1} \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2v}} \frac{\delta_{l,\gamma}(\mathbf{x})}{n^l} + \sum_{l=v+1}^{2v} \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2v+1}} \frac{\delta_{l,\gamma}(\mathbf{x})}{n^l} \\
 &= \frac{d_{1,v+1}(\mathbf{x})}{n} + \dots + \frac{d_{v,v+1}(\mathbf{x})}{n^v} + \frac{d_{v+1,v+1}(\mathbf{x})}{n^{v+1}} + O(n^{-(v+2)})
 \end{aligned}$$

and comparing coefficients on both sides of this equation proves the claim.

We now define, for $v = 1, \dots, k$, coefficient functions $\tilde{c}_v(\mathbf{x})$ by

$$\tilde{c}_v(\mathbf{x}) := d_{v,v}(\mathbf{x}) + \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2v}} \frac{1}{\gamma!} \delta_{v,\gamma}(\mathbf{x}) D^\gamma f(\mathbf{x}). \tag{21}$$

We now claim: For $m = 1, \dots, k$, it is

$$\lim_{n \rightarrow \infty} n^m \left\{ B_n(f; \mathbf{x}) - f(\mathbf{x}) - \sum_{v=1}^{m-1} \frac{\tilde{c}_v(\mathbf{x})}{n^v} \right\} = \tilde{c}_m(\mathbf{x}). \tag{22}$$

For $m = 1$, this was established in [3] as a corollary to Theorem 3.

Now let $2 \leq m \leq k$. From (19) in connection with Theorem 4, we get

$$\begin{aligned}
 &\lim_{n \rightarrow \infty} n^m \left(B_n(f; \mathbf{x}) - f(\mathbf{x}) - \left(\frac{d_{1,m}(\mathbf{x})}{n} + \dots + \frac{d_{m,m}(\mathbf{x})}{n^m} \right) \right) \\
 &= \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2m}} \frac{1}{\gamma!} \sum_{\substack{\beta^1, \dots, \beta^m \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^m = \gamma}} \prod_{i=1}^m \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) D^\gamma f(\mathbf{x}). \\
 &\hspace{10em} |\beta^i| \geq 2, i=1, \dots, m
 \end{aligned}$$

Together with (21), (20) and (18), this gives

$$\lim_{n \rightarrow \infty} n^m \left(B_n(f; \mathbf{x}) - f(\mathbf{x}) - \sum_{v=1}^{m-1} \frac{\tilde{c}_v(\mathbf{x})}{n^v} - \frac{d_{m,m}(\mathbf{x})}{n^m} \right) = \sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma|=2m}} \frac{1}{\gamma!} \delta_{v,\gamma}(\mathbf{x}) D^\gamma f(\mathbf{x}),$$

and so, using (21) once more, (22) is proved.

This also completes the proof of the existence of the asymptotic expansion, as stated in (10).

To verify (11) (i.e., to prove that $c_v = \tilde{c}_v$), we once again analyse the sum in (19). Using (16) gives

$$\sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma| \leq 2v-1}} \frac{1}{\gamma!} \sum_{\mu=1}^{\lfloor \frac{|\gamma|}{2} \rfloor} \sum_{i=1}^{\mu} \frac{\alpha_{i,\mu}}{n^{|\gamma|-i}} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) D^\gamma f(\mathbf{x}).$$

Table 1a
Errors in approximating f_1

0.2083e(00)			
0.9896e(-1)	0.1042e(-1)	0.5208e(-2)	
0.4622e(-1)	0.6510e(-2)	0.6510e(-3)	0.0000e(1)
0.2205e(-1)	0.2116e(-2)	0.8138e(-4)	0.0000e(1)
0.1073e(-1)	0.5900e(-3)	0.1017e(-4)	0.0000e(1)
0.5288e(-2)	0.1551e(-3)	0.1272e(-5)	0.0000e(1)
0.2624e(-2)	0.3974e(-4)		

Table 1b
Quotients of the entries of Table 1a

2.105	1.600	
2.141	3.077	8.000
2.096	3.586	8.000
2.055	3.803	8.000
2.029	3.904	8.000
2.015	3.953	8.000
2.008		

Collecting in this expression all terms containing $1/n^v$ shows that the coefficient of this power of n is

$$\sum_{\substack{\gamma \in \mathbb{N}_0^s \\ |\gamma| \leq 2v-1}} \frac{1}{\gamma!} \sum_{\mu=1}^{\lfloor \frac{|\gamma|}{2} \rfloor} \alpha_{|\gamma|-v, \mu} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) D^\gamma f(\mathbf{x}).$$

Since $\alpha_{i, \mu} = 0$ for $i \leq 0$ and $i > \mu$, this is equal to

$$\sum_{\substack{\gamma \in \mathbb{N}_0^s \\ v+1 \leq |\gamma| \leq 2v-1}} \frac{1}{\gamma!} \sum_{\mu=|\gamma|-v}^{\lfloor \frac{|\gamma|}{2} \rfloor} \alpha_{|\gamma|-v, \mu} \sum_{\substack{\beta^1, \dots, \beta^\mu \in \mathbb{N}_0^s \\ \beta^1 + \dots + \beta^\mu = \gamma \\ |\beta^i| \geq 2, i=1, \dots, \mu}} \prod_{i=1}^{\mu} \left(\sum_{j=0}^s \lambda_j (v^j - \mathbf{x})^{\beta^i} \right) D^\gamma f(\mathbf{x}).$$

Now using once more relation (18) completes the proof of Theorem 5. \square

Table 2a
Errors in approximating f_2

0.1097e(00)				
	0.2113e(-2)			
0.5378e(-1)		0.1500e(-4)		
	0.5396e(-3)		0.2869e(-6)	
0.2662e(-1)		0.1624e(-5)		0.1575e(-9)
	0.1361e(-3)		0.1779e(-7)	
0.1324e(-1)		0.1875e(-6)		0.7047e(-11)
	0.3417e(-4)		0.1105e(-8)	
0.6603e(-2)		0.2247e(-7)		0.2520e(-12)
	0.8559e(-5)		0.6883e(-10)	
0.3297e(-2)		0.2748e(-8)		0.8359e(-14)
	0.2142e(-5)		0.4294e(-11)	
0.1648e(-2)		0.3398e(-9)		0.2687e(-15)
	0.5357e(-6)		0.2681e(-12)	
0.8235e(-3)		0.4224e(-10)		
	0.1340e(-6)			
0.4117e(-3)				

Table 2b
Quotients of the entries of Table 2a

2.039				
	3.917			
2.020		9.237		
	3.964		16.133	
2.010		8.664		22.345
	3.984		16.096	
2.005		8.344		27.966
	3.992		16.055	
2.003		8.175		30.146
	3.996		16.029	
2.001		8.088		31.111
	3.998		16.015	
2.001		8.044		
	3.999			
2.000				

3. Numerical results

Having proved the existence of the asymptotic expansion (10), we can now apply the extrapolation process (4) to the sequence of Bernstein approximants. It follows from (10) that $\rho_k = k$ for all k . In order to illustrate the numerical effect of extrapolation, we show in this section a small selection of a number of numerical tests that have been examined, and all of which showed the asymptotic behaviour that was predicted.

The results shown below were obtained for $s = 2$ on the triangle T with vertices

$$v^0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad v^1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad v^2 = \begin{pmatrix} 0 \\ 2 \end{pmatrix}$$

in euclidean coordinates. We computed the absolute values of the error functions in the barycenter of T , the point

$$\beta = \frac{1}{3}(v^0 + v^1 + v^2).$$

As a first test, we applied the method to the bivariate polynomial

$$f_1(x, y) := xy^3.$$

The errors of the approximations $y_i^{(k)}$ of the true value $f_1(\beta) = \frac{1}{3}$, computed by extrapolation with $K=3$, $n_0=2$, and $i=0, \dots, 6$, are shown in Table 1a. As expected, the entries of the third column are identically zero, since f_1 is a polynomial of total degree 4, and therefore the third extrapolation step already gives the exact result. Note in this connection that the Bernstein approximants themselves do *not* reproduce the polynomial f_1 exactly, however high their degree might be.

As a second example, we consider approximation of the function

$$f_2(x, y) := \exp(x + y)$$

and again compare our numerical approximations with the true value of f_2 in β , which is $\exp(\frac{4}{3})$. This time, the errors (in absolute value) of the approximations computed by our method with $K=4$, $n_0=4$, and $i=0, \dots, 8$ are shown, see Table 2a.

In Tables 1b and 2b, finally, we have the *quotients* of two subsequent values in the columns of Table 1a (resp. Table 2a). As predicted, the entries of the k th column (starting to count with $k=0$) converge to 2^{k+1} .

4. Conclusion

In contrast to the univariate case, the approximation of multivariate functions by polynomials is still a very difficult task, and many problems are open. Up to now, there exist very few numerical methods for the computation of good polynomial approximations. Therefore, we are convinced that the approach developed in this paper provides a very efficient new method for polynomial approximation of multivariate functions.

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Prediction properties of Aitken's iterated Δ^2 process, of Wynn's epsilon algorithm, and of Brezinski's iterated theta algorithm

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Abstract

The prediction properties of Aitken's iterated Δ^2 process, Wynn's epsilon algorithm, and Brezinski's iterated theta algorithm for (formal) power series are analyzed. As a first step, the defining recursive schemes of these transformations are suitably rearranged in order to permit the derivation of accuracy-through-order relationships. On the basis of these relationships, the rational approximants can be rewritten as a partial sum plus an appropriate transformation term. A Taylor expansion of such a transformation term, which is a rational function and which can be computed recursively, produces the predictions for those coefficients of the (formal) power series which were not used for the computation of the corresponding rational approximant. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

In applied mathematics and in theoretical physics, Padé approximants are now used almost routinely to overcome problems with slowly convergent or divergent power series. Of course, there is an extensive literature on Padé approximants: In addition to countless articles, there are several textbooks [4,5,8,17,28,41,44,52,73], review articles [3,6,9,24,25,55,119], collections of articles and proceedings [7,21,29,39,40,42,53,56–58,78,112,114], bibliographies [14,20,115], and there is even a book [19] and an article [22], respectively, treating the history of Padé approximants and related topics. A long but by no means complete list of applications of Padé approximants in physics and chemistry can be found in Section 4 of Weniger [100].

The revival of the interest in Padé approximants was initiated by two articles by Shanks [84] and Wynn [116], respectively. These articles, which stimulated an enormous amount of research, were published in 1956 at a time when electronic computers started to become more widely available. Shanks [84] introduced a sequence transformation which produces Padé approximants if the input

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data are the partial sums of a power series, and Wynn [116] showed that this transformation can be computed conveniently and effectively by a recursive scheme now commonly called the epsilon algorithm. As a consequence of the intense research initiated by Shanks [84] and Wynn [116], the mathematical properties of Padé approximants are now fairly well understood, and it is generally accepted that Padé approximants are extremely useful numerical tools which can be applied profitably in a large variety of circumstances.

This intense research of course also showed that Padé approximants have certain limitations and shortcomings. For example, Padé approximants are in principle limited to convergent and divergent power series and cannot help in the case of many other slowly convergent sequences and series with different convergence types.

The convergence type of numerous practically important sequences $\{s_n\}_{n=0}^\infty$ can be classified by the asymptotic condition

$$\lim_{n \rightarrow \infty} \frac{s_{n+1} - s}{s_n - s} = \rho, \tag{1.1}$$

which closely resembles the well-known ratio test for infinite series. Here, $s = s_\infty$ is the limit of $\{s_n\}_{n=0}^\infty$ as $n \rightarrow \infty$. A convergent sequence satisfying (1.1) with $|\rho| < 1$ is called *linearly* convergent, and it is called *logarithmically* convergent if $\rho = 1$. The partial sums of a power series with a nonzero, but finite radius of convergence are a typical example of a linearly convergent sequence. The partial sums of the Dirichlet series for the Riemann zeta function

$$\zeta(z) = \sum_{m=0}^\infty (m+1)^{-z}, \quad \text{Re}(z) > 1, \tag{1.2}$$

which is notorious for its extremely slow convergence if $\text{Re}(z)$ is only slightly larger than one, are a typical example of a logarithmically convergent sequence.

Padé approximants as well as the closely related epsilon algorithm [116] are known to accelerate effectively the convergence of linearly convergent power series and they are also able to sum many divergent power series. However, they fail completely in the case of logarithmic convergence (compare for example [117, Theorem 12]). Moreover, in the case of divergent power series whose series coefficients grow more strongly than factorially, Padé approximants either converge too slowly to be numerically useful [35,86] or are not at all able to accomplish a summation to a unique finite generalized limit [54]. Consequently, the articles by Shanks [84] and Wynn [116] also stimulated research on sequence transformations. The rapid progress in this field is convincingly demonstrated by the large number of monographs and review articles on sequence transformations which appeared in recent years [15,16,23,26,43,67,70,94,95,113].

In some, but by no means in all cases, sequence transformations are able to do better than Padé approximants, and it may even happen that they clearly outperform Padé approximants. Thus, it may well be worth while to investigate whether it is possible to use instead of Padé approximants more specialized sequence transformations which may be better adapted to the problem under consideration. For example, the present author used sequence transformations successfully as computational tools in such diverse fields as the evaluation of special functions [61,63,95,96,99,100,103,106], the evaluation of molecular multicenter integrals of exponentially decaying functions [59,90,100,109,111], the summation of strongly divergent quantum mechanical perturbation expansions [33,34,36,96,98, 100–102,104,105,107,108], and the extrapolation of quantum chemical ab initio calculations for

oligomers to the infinite chain limit of quasi-one-dimensional stereoregular polymers [32,100,110]. In vast majority of these applications, it was either not possible to use Padé approximants at all, or alternative sequence transformations did a better job.

In most practical applications of Padé approximants or also of sequence transformations, the partial sums of (formal) power series are transformed into rational approximants with the intention of either accelerating convergence or to accomplish a summation to a finite (generalized) limit in the case of divergence. Padé approximants and sequence transformations are normally not used for the computation of the coefficients of the power series. In the majority of applications, the computation of the coefficients of power series is not the most serious computational problem, and conventional methods for the computation of the coefficients usually suffice.

However, in the case of certain perturbation expansions as they for instance occur in high energy physics, in quantum field theory, or in quantum chromodynamics, the computational problems can be much more severe. Not only do these perturbation expansions, which are power series in some coupling constant, diverge quite strongly for every nonzero value of the coupling constant, but it is also extremely difficult to compute more than just a few of the perturbation series coefficients. Moreover, due to the complexity of the computations and the necessity of making often drastic approximations, the perturbation series coefficients obtained in this way are usually affected by comparatively large relative errors. Under such adverse circumstances, it has recently become customary to use Padé approximants to make predictions about the leading unknown coefficients of perturbation expansions as well as to make consistency checks for the previously calculated coefficients [27,30,31,46–50,65, 79–83,89].

On a heuristic level, the prediction capability of Padé approximants, which was apparently first used by Gilewicz [51], can be explained quite easily. Let us assume that a function f possesses the following (formal) power series:

$$f(z) = \sum_{v=0}^{\infty} \gamma_v z^v \quad (1.3)$$

and that we want to transform the sequence of its partial sums

$$f_n(z) = \sum_{v=0}^n \gamma_v z^v \quad (1.4)$$

into a doubly indexed sequence of Padé approximants

$$[l/m]_f(z) = P_l(z)/Q_m(z). \quad (1.5)$$

As is well known [4,8], the coefficients of the polynomials $P_l(z) = p_0 + p_1z + \cdots + p_lz^l$ and $Q_m(z) = 1 + q_1z + \cdots + q_mz^m$ are chosen in such a way that the Taylor expansion of the Padé approximant agrees as far as possible with the (formal) power series (1.3):

$$f(z) - P_l(z)/Q_m(z) = O(z^{l+m+1}), \quad z \rightarrow 0. \quad (1.6)$$

This *accuracy-through-order* relationship implies that the Padé approximant to $f(z)$ can be written as the partial sum, from which it was constructed, plus a term which was generated by the transformation of the partial sum to the rational approximant:

$$[l/m]_f(z) = \sum_{v=0}^{l+m} \gamma_v z^v + z^{l+m+1} \mathcal{P}_l^m(z) = f_{l+m}(z) + z^{l+m+1} \mathcal{P}_l^m(z). \quad (1.7)$$

Similarly, the (formal) power series (1.3) can be expressed as follows:

$$f(z) = \sum_{v=0}^{l+m} \gamma_v z^v + z^{l+m+1} \mathcal{F}_{l+m+1}(z) = f_{l+m}(z) + z^{l+m+1} \mathcal{F}_{l+m+1}(z). \tag{1.8}$$

Let us now assume that the Padé approximant $[l/m]_f(z)$ provides a sufficiently accurate approximation to $f(z)$. Then, the Padé transformation term $\mathcal{P}_l^m(z)$ must also provide a sufficiently accurate approximation to the truncation error $\mathcal{F}_{l+m+1}(z)$ of the (formal) power series. In general, we have no reason to assume that $\mathcal{P}_l^m(z)$ could be equal to $\mathcal{F}_{l+m+1}(z)$ for finite values of l and m . Consequently, Taylor expansions of $\mathcal{P}_l^m(z)$ and $\mathcal{F}_{l+m+1}(z)$, respectively, will in general produce different results. Nevertheless, the *leading* coefficients of the Taylor expansion for $\mathcal{P}_l^m(z)$ should provide sufficiently accurate approximations to the corresponding coefficients of the Taylor series for $\mathcal{F}_{l+m+1}(z)$.

It is important to note that this prediction capability does not depend on the convergence of the power series expansions for $\mathcal{P}_l^m(z)$ and $\mathcal{F}_{l+m+1}(z)$, respectively. Padé approximants are able to make predictions about series coefficients even if the power series (1.3) for f as well as the power series expansions for \mathcal{P}_l^m and $\mathcal{F}_{l+m+1}(z)$ are only asymptotic as $z \rightarrow 0$. This fact explains why the prediction capability of Padé approximants can be so very useful in the case of violently divergent perturbation expansions.

Let us now assume that a sequence transformation also produces a convergent sequence of rational approximants if it acts on the partial sums (1.4) of the (formal) power series (1.3). Then, by the same line of reasoning, these rational approximants should also be able to make predictions about the leading coefficients of the power series, which were not used for the construction of the rational approximant. It seems that these ideas were first formulated by Sidi and Levin [85] and Brezinski [18]. Recently, these ideas were extended by Prévost and Vekemans [72] who discussed prediction methods for sequences which they called ε_p and partial Padé prediction, respectively. Moreover, in [105] it was shown that suitably chosen sequence transformations can indeed make more accurate predictions about unknown power series coefficients than Padé approximants.

Consequently, it should be interesting to analyze the prediction properties of sequence transformations. In this this article, only Aitken’s iterated Δ^2 algorithm, Wynn’s epsilon algorithm and the iteration of Brezinski’s theta algorithm will be considered. Further studies on the prediction properties of other sequence transformations are in progress and will be presented elsewhere.

If the prediction properties of sequence transformations are to be studied, there is an additional complication which is absent in the case of Padé approximants. The accuracy-through-order relationship (1.6) leads to a system of $l + m + 1$ linear equations for the coefficients of the polynomials $P_l(z) = p_0 + p_1z + \dots + p_lz^l$ and $Q_m(z) = 1 + q_1z + \dots + q_mz^m$ of the Padé approximant (1.5) [5,8]. If this system of equations has a solution, then it is automatically guaranteed that the Padé approximant obtained in this way satisfies the accuracy-through-order relationship (1.6).

In the case of the sequence transformations considered in this article, the situation is in general more complicated. These transformations are not defined as solutions of systems of linear equations, but via nonlinear recursive schemes. Moreover, their accuracy-through-order relationships are with the exception of Wynn’s epsilon algorithm unknown and have to be derived via their defining recursive schemes.

On the basis of these accuracy-through-order relationships, it is possible to construct explicit recursive schemes for the transformation errors as well as for the first coefficient of the power series which was not used for the computation of the rational approximant.

In Section 2, the accuracy-through-order and prediction properties of Aitken's iterated Δ^2 process are analyzed. In Section 3, the analogous properties of Wynn's epsilon algorithm are discussed, and in Section 4, Brezinski's iterated theta algorithm is treated. In Section 5, some applications of the new results are presented. This article is concluded by Section 6 which contains a short summary.

2. Aitken's iterated Δ^2 process

Let us consider the following model sequence:

$$s_n = s + c\lambda^n, \quad c \neq 0, \quad |\lambda| \neq 1, \quad n \in \mathbb{N}_0. \quad (2.1)$$

For $n \rightarrow \infty$, this sequence obviously converges to its limit s if $0 < |\lambda| < 1$, and it diverges away from its generalized limit s if $|\lambda| > 1$.

A sequence transformation, which is able to determine the (generalized) limit s of the model sequence (2.1) from the numerical values of three consecutive sequence elements s_n , s_{n+1} and s_{n+2} , can be constructed quite easily. Just consider s , c , and λ as unknowns of the linear system $s_{n+j} = s + c\lambda^{n+j}$ with $j = 0, 1, 2$. A short calculation shows that

$$\mathcal{A}_1^{(n)} = s_n - \frac{[\Delta s_n]^2}{\Delta^2 s_n}, \quad n \in \mathbb{N}_0 \quad (2.2)$$

is able to determine the (generalized) limit of the model sequence (2.1) according to $\mathcal{A}_1^{(n)} = s$. It should be noted that s can be determined in this way, no matter whether sequence (2.1) converges or diverges. The forward difference operator Δ in (2.2) is defined by its action on a function $g = g(n)$:

$$\Delta g(n) = g(n+1) - g(n). \quad (2.3)$$

The Δ^2 formula (2.2) is certainly one of the oldest sequence transformations. It is usually attributed to Aitken [1], but it is actually much older. Brezinski [19, pp. 90–91] mentioned that in 1674 Seki Kowa, the probably most famous Japanese mathematician of that period, tried to obtain better approximations to π with the help of this Δ^2 formula, and according to Todd [91, p. 5] it was in principle already known to Kummer [66].

There is an extensive literature on Aitken's Δ^2 process. For example, it was discussed by Lubkin [68], Shanks [84], Tucker [92,93], Clark et al. [37], Cordellier [38], Jurkat [64], Bell and Phillips [10], and Weniger [95, Section 5]. A multidimensional generalization of Aitken's transformation to vector sequences was discussed by MacLeod [69]. Modifications and generalizations of Aitken's Δ^2 process were proposed by Drummond [45], Jamieson and O'Beirne [62], Bjørstad et al. [12], and Sablonniere [76]. Then, there is a close connection between the Aitken process and Fibonacci numbers, as discussed by McCabe and Phillips [71] and Arai et al. [2]. The properties of Aitken's Δ^2 process are also discussed in books by Baker and Graves-Morris [8], Brezinski [15,16], Brezinski and Redivo Zaglia [26], Delahaye [43], Walz [94], and Wimp [113].

The power of Aitken's Δ^2 process is of course limited since it is designed to eliminate only a single exponential term. However, its power can be increased considerably by iterating it, yielding the following nonlinear recursive scheme:

$$\mathcal{A}_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \quad (2.4a)$$

$$\mathcal{A}_{k+1}^{(n)} = \mathcal{A}_k^{(n)} - \frac{[\Delta \mathcal{A}_k^{(n)}]^2}{\Delta^2 \mathcal{A}_k^{(n)}}, \quad k, n \in \mathbb{N}_0. \quad (2.4b)$$

In the case of doubly indexed quantities like $\mathcal{A}_k^{(n)}$, it will always be assumed that the difference operator Δ only acts on the superscript n but not on the subscript k :

$$\Delta \mathcal{A}_k^{(n)} = \mathcal{A}_k^{(n+1)} - \mathcal{A}_k^{(n)}. \tag{2.5}$$

The numerical performance of Aitken’s iterated Δ^2 process was studied in [88,95]. Concerning the theoretical properties of Aitken’s iterated Δ^2 process, very little seems to be known. Hillion [60] was able to find a model sequence for which the iterated Δ^2 process is exact. He also derived a determinantal representation for $\mathcal{A}_k^{(n)}$. However, Hillion’s expressions for $\mathcal{A}_k^{(n)}$ contain explicitly the lower order transforms $\mathcal{A}_0^{(n)}, \dots, \mathcal{A}_{k-1}^{(n)}, \dots, \mathcal{A}_0^{(n+k)}, \dots, \mathcal{A}_{k-1}^{(n+k)}$. Consequently, it seems that Hillion’s result [60] — although interesting from a formal point of view — cannot help much to analyze the prediction properties of $\mathcal{A}_k^{(n)}$.

If we want to use Aitken’s iterated Δ^2 process for the prediction of unknown series coefficients, we first have to derive its accuracy-through-order relationship of the type of (1.6) on the basis of the recursive scheme (2.4).

It is a direct consequence of the recursive scheme (2.4) that $2k + 1$ sequence elements $s_n, s_{n+1}, \dots, s_{n+2k}$ are needed for the computation of $\mathcal{A}_k^{(n)}$. Thus, we now choose as input data the partial sums (1.4) of the (formal) power series (1.3) according to $s_n = f_n(z)$, and conjecture that all coefficients $\gamma_0, \gamma_1, \dots, \gamma_{n+2k}$, which were used for the construction of $\mathcal{A}_k^{(n)}$, are exactly reproduced by a Taylor expansion. This means that we have to look for an accuracy-through-order relationship of the following kind:

$$f(z) - \mathcal{A}_k^{(n)} = O(z^{n+2k+1}), \quad z \rightarrow 0. \tag{2.6}$$

Such an accuracy-through-order relationship would imply that $\mathcal{A}_k^{(n)}$ can be expressed as follows:

$$\mathcal{A}_k^{(n)} = f_{n+2k}(z) + G_k^{(n)} z^{n+2k+1} + O(z^{n+2k+2}), \quad z \rightarrow 0. \tag{2.7}$$

The constant $G_k^{(n)}$ is the prediction made for the coefficient γ_{n+2k+1} , which is the first coefficient of the power series (1.3) not used for the computation of $\mathcal{A}_k^{(n)}$.

Unfortunately, the recursive scheme (2.4) is not suited for our purposes. This can be shown by computing $\mathcal{A}_1^{(n)}$ from the partial sums $f_n(z), f_{n+1}(z)$, and $f_{n+2}(z)$:

$$\mathcal{A}_1^{(n)} = f_n(z) + \frac{[\gamma_{n+1}]^2 z^{n+1}}{\gamma_{n+1} - \gamma_{n+2} z}. \tag{2.8}$$

Superficially, it looks as if $\mathcal{A}_1^{(n)}$ is not of the type of (2.7). However, the rational expression on the right-hand side contains the missing terms $\gamma_{n+1} z^{n+1}$ and $\gamma_{n+2} z^{n+2}$. We only have to use $1/(1 - y) = 1 + y + y^2/(1 - y)$ with $y = \gamma_{n+2} z / \gamma_{n+1}$ to obtain an equivalent expression with the desired features:

$$\mathcal{A}_1^{(n)} = f_{n+2}(z) + \frac{[\gamma_{n+2}]^2 z^{n+3}}{\gamma_{n+1} - \gamma_{n+2} z}. \tag{2.9}$$

Thus, an expression, which is in agreement with (2.7), can be obtained easily in the case of the simplest transform $\mathcal{A}_1^{(n)}$. Moreover, (2.9) makes the prediction $G_1^{(n)} = [\gamma_{n+2}]^2 / \gamma_{n+1}$ for the first series coefficient γ_{n+3} not used for the computation of $\mathcal{A}_1^{(n)}$. Of course, by expanding the denominator on the right-hand side of (2.9) further predictions on series coefficients with higher indices can be made.

In the case of more complicated transforms $\mathcal{A}_k^{(n)}$ with $k > 1$, it is by no means obvious whether and how the necessary manipulations, which would transform an expression of the type of (2.8)

into an expression of the type of (2.9), can be done. Consequently, it is advantageous to replace the recursive scheme (2.4) by an alternative recursive scheme, which directly leads to appropriate expressions for $\mathcal{A}_k^{(n)}$ with $k > 1$.

Many different expressions for $\mathcal{A}_1^{(n)}$ in terms of s_n , s_{n+1} , and s_{n+2} are known [95, Section 5.1]. These expressions are all mathematically equivalent although their numerical properties may differ. Comparison with (2.9) shows that the for our purposes appropriate expression is [95, Eq. (5.1-7)]

$$\mathcal{A}_1^{(n)} = s_{n+2} - \frac{[\Delta s_{n+1}]^2}{\Delta^2 s_n}. \tag{2.10}$$

Just like (2.2), this expression can be iterated and yields

$$\mathcal{A}_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{2.11a}$$

$$\mathcal{A}_{k+1}^{(n)} = \mathcal{A}_k^{(n+2)} - \frac{[\Delta \mathcal{A}_k^{(n+1)}]^2}{\Delta^2 \mathcal{A}_k^{(n)}}, \quad k, n \in \mathbb{N}_0. \tag{2.11b}$$

The recursive schemes (2.4) and (2.11) are mathematically completely equivalent. However, for our purposes — the analysis of the prediction properties of Aitken’s iterated Δ^2 process in the case of power series — the recursive scheme (2.11) is much better suited.

Next, we rewrite the partial sums (1.4) of the (formal) power series (1.3) according to

$$f_n(z) = f(z) - \sum_{v=0}^{\infty} \gamma_{n+v+1} z^{n+v+1} \tag{2.12}$$

and use them as input data in the recursive scheme (2.11). This yields the following expression:

$$\mathcal{A}_k^{(n)} = f(z) + z^{n+2k+1} R_k^{(n)}(z), \quad k, n \in \mathbb{N}_0. \tag{2.13}$$

The quantities $R_k^{(n)}(z)$ can be computed with the help of the following recursive scheme which is a direct consequence of the recursive scheme (2.11) for $\mathcal{A}_k^{(n)}$:

$$R_0^{(n)}(z) = - \sum_{v=0}^{\infty} \gamma_{n+v+1} z^v = \frac{f_n(z) - f(z)}{z^{n+1}}, \quad n \in \mathbb{N}_0, \tag{2.14a}$$

$$R_{k+1}^{(n)}(z) = R_k^{(n+2)}(z) - \frac{[\delta R_k^{(n+1)}(z)]^2}{\delta^2 R_k^{(n)}(z)}, \quad k, n \in \mathbb{N}_0. \tag{2.14b}$$

In (2.14), we use the shorthand notation

$$\delta X_k^{(n)}(z) = z X_k^{(n+1)}(z) - X_k^{(n)}(z), \tag{2.15a}$$

$$\begin{aligned} \delta^2 X_k^{(n)}(z) &= z \delta X_k^{(n+1)}(z) - \delta X_k^{(n)}(z) \\ &= z^2 X_k^{(n+2)}(z) - 2z X_k^{(n+1)}(z) + X_k^{(n)}(z). \end{aligned} \tag{2.15b}$$

It seems that we have now accomplished our aim since (2.13) has the right structure to serve as an accuracy-through-order relationship for Aitken’s iterated Δ^2 process. Unfortunately, this conclusion is in general premature and we have to require that the input data satisfy some additional conditions. One must not forget that Aitken’s Δ^2 formula (2.10) as well as its iteration (2.11) cannot be applied to arbitrary input data. One obvious potential complication, which has to be excluded, is that (2.11b)

becomes undefined if $\Delta^2 \mathcal{A}_k^{(n)} = 0$. Thus, if we want to transform the partial sums (1.4) of the (formal) power series (1.3), it is natural to require that all series coefficients are nonzero, i.e., $\gamma_v \neq 0$ for all $v \in \mathbb{N}_0$.

Unfortunately, this is only a minimal requirement and not yet enough for our purposes. If $z^{n+2k+1}R_k^{(n)}(z)$ in (2.13) is to be of order $O(z^{n+2k+1})$ as $z \rightarrow 0$, then the z -independent part $C_k^{(n)}$ of $R_k^{(n)}(z)$ defined by

$$R_k^{(n)}(z) = C_k^{(n)} + O(z), \quad z \rightarrow 0, \tag{2.16}$$

has to satisfy

$$C_k^{(n)} \neq 0, \quad k, n \in \mathbb{N}_0. \tag{2.17}$$

If these conditions are satisfied, we can be sure that (2.13) is indeed the accuracy-through-order relationship we have been looking for.

Personally, I am quite sceptical that it would be easy to characterize *theoretically* those power series which give rise to truncation errors $R_k^{(n)}(z)$ satisfying (2.16) and (2.17). Fortunately, it can easily be checked *numerically* whether a given (formal) power series leads to truncation errors whose z -independent parts are nonzero. If we set $z = 0$ in (2.14) and use (2.16), we obtain the following recursive scheme:

$$C_0^{(n)} = -\gamma_{n+1}, \quad n \in \mathbb{N}_0, \tag{2.18a}$$

$$C_{k+1}^{(n)} = C_k^{(n+2)} - \frac{[C_k^{(n+1)}]^2}{C_k^{(n)}}, \quad k, n \in \mathbb{N}_0. \tag{2.18b}$$

Let us now assume that we know for a given (formal) power series that the z -independent parts $C_k^{(n)}$ of the truncation errors $R_k^{(n)}(z)$ in (2.13) are nonzero — either from a mathematical proof or from a brute force calculation using (2.18). Then, (2.13) is indeed the accuracy-through-order relationship we have been looking for, which implies that $\mathcal{A}_k^{(n)}$ can be expressed as follows:

$$\mathcal{A}_k^{(n)} = f_{n+2k}(z) + z^{n+2k+1}\Phi_k^{(n)}(z), \quad k, n \in \mathbb{N}_0. \tag{2.19}$$

If we use this ansatz in (2.11), we obtain the following recursive scheme:

$$\Phi_0^{(n)}(z) = 0, \quad n \in \mathbb{N}_0, \tag{2.20a}$$

$$\Phi_{k+1}^{(n)}(z) = \Phi_k^{(n+2)}(z) - \frac{[\gamma_{n+2k+2} + \delta\Phi_k^{(n+1)}(z)]^2}{\gamma_{n+2k+2z} - \gamma_{n+2k+1} + \delta^2\Phi_k^{(n)}(z)}, \quad k, n \in \mathbb{N}_0. \tag{2.20b}$$

Here, $\delta\Phi_k^{(n)}(z)$ and $\delta^2\Phi_k^{(n)}(z)$ are defined by (2.15). For $k = 0$, (2.20b) yields

$$\Phi_1^{(n)}(z) = \frac{[\gamma_{n+2}]^2}{\gamma_{n+1} - \gamma_{n+2z}}, \tag{2.21}$$

which is in agreement with (2.9).

A comparison of (2.7) and (2.19) yields

$$\Phi_k^{(n)}(z) = G_k^{(n)} + O(z), \quad z \rightarrow 0. \tag{2.22}$$

Consequently, the z -independent part $G_k^{(n)}$ of $\Phi_k^{(n)}(z)$ is the prediction for the first coefficient γ_{n+2k+1} not used for the computation of $\mathcal{A}_k^{(n)}$.

If we set $z = 0$ in the recursive scheme (2.20) and use (2.22), we obtain the following recursive scheme for the predictions $G_k^{(n)}$:

$$G_0^{(n)} = 0, \quad n \in \mathbb{N}_0, \tag{2.23a}$$

$$G_1^{(n)} = [\gamma_{n+2}]^2 / \gamma_{n+1}, \quad n \in \mathbb{N}_0, \tag{2.23b}$$

$$G_{k+1}^{(n)} = G_k^{(n+2)} + \frac{[\gamma_{n+2k+2} - G_k^{(n+1)}]^2}{\gamma_{n+2k+1} - G_k^{(n)}}, \quad k, n \in \mathbb{N}_0. \tag{2.23c}$$

The z -independent parts $C_k^{(n)}$ of $R_k^{(n)}(z)$ and $G_k^{(n)}$ of $\Phi_k^{(n)}(z)$, respectively, are connected. A comparison of (2.13), (2.16), (2.19), and (2.22) yields

$$G_k^{(n)} = C_k^{(n)} + \gamma_{n+2k+1}. \tag{2.24}$$

In this article, rational approximants will always be used in such a way that the input data — the partial sums (1.4) of the (formal) power series (1.3) — are computed in an outer loop, and for each new partial sum a new approximation to the limit is calculated. If the index m of the last partial sum $f_m(z)$ is even, $m = 2\mu$, we use in the case of Aitken’s iterated Δ^2 process as approximation to the limit $f(z)$ the transformation

$$\{f_0(z), f_1(z), \dots, f_{2\mu}(z)\} \mapsto \mathcal{A}_\mu^{(0)}, \tag{2.25}$$

and if m is odd, $m = 2\mu + 1$, we use the transformation

$$\{f_1(z), f_2(z), \dots, f_{2\mu+1}(z)\} \mapsto \mathcal{A}_\mu^{(1)}. \tag{2.26}$$

With the help of the notation $\llbracket x \rrbracket$ for the integral part of x , which is the largest integer v satisfying the inequality $v \leq x$, these two relationships can be combined into a single equation, yielding [95, Eq. (5.2–6)]

$$\{f_{m-2\llbracket m/2 \rrbracket}(z), f_{m-2\llbracket m/2 \rrbracket+1}(z), \dots, f_m(z)\} \mapsto \mathcal{A}_{\llbracket m/2 \rrbracket}^{(m-2\llbracket m/2 \rrbracket)}, \quad m \in \mathbb{N}_0. \tag{2.27}$$

The same strategy will also be used if for example the rational expressions $R_k^{(n)}(z)$ defined by (2.13) are listed in a table. This means that the $R_k^{(n)}(z)$ will also be listed according to (2.27). The only difference is that the $R_k^{(n)}(z)$ use as input data not the partial sums $f_n(z)$ but the remainders $[f_n(z) - f(z)]/z^{n+1}$.

3. Wynn’s epsilon algorithm

Wynn’s epsilon algorithm [116] is the following nonlinear recursive scheme:

$$\varepsilon_{-1}^{(n)} = 0, \quad \varepsilon_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{3.1a}$$

$$\varepsilon_{k+1}^{(n)} = \varepsilon_{k-1}^{(n+1)} + 1/[\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}], \quad k, n \in \mathbb{N}_0. \tag{3.1b}$$

The elements $\varepsilon_{2k}^{(n)}$ with *even* subscripts provide approximations to the (generalized) limit s of the sequence $\{s_n\}_{n=0}^\infty$ to be transformed, whereas the elements $\varepsilon_{2k+1}^{(n)}$ with *odd* subscripts are only auxiliary quantities which diverge if the whole process converges.

If the input data are the partial sums (1.4) of the (formal) power series (1.3), $s_n = f_n(z)$, then Wynn [116] could show that his epsilon algorithm produces Padé approximants

$$\varepsilon_{2k}^{(n)} = [n + k/k]_f(z). \tag{3.2}$$

The epsilon algorithm is a close relative of Aitken’s iterated Δ^2 process, and they have similar properties in convergence acceleration and summation processes. A straightforward calculation shows that $\mathcal{A}_1^{(n)} = \varepsilon_2^{(n)}$. Hence, Aitken’s iterated Δ^2 process may also be viewed as an iteration of $\varepsilon_2^{(n)}$. However, for $k > 1$, $\mathcal{A}_k^{(n)}$ and $\varepsilon_{2k}^{(n)}$ are in general different.

There is an extensive literature on the epsilon algorithm. On p. 120 of Wimps book [113] it is mentioned that over 50 articles on the epsilon algorithm were published by Wynn alone, and at least 30 articles by Brezinski. As a fairly complete source of references Wimp recommends Brezinski’s first book [15]. However, this book was published in 1977, and since then many more articles on the epsilon algorithm have been published. Consequently, any attempt to produce something resembling a reasonably complete bibliography of Wynn’s epsilon algorithm would clearly be beyond the scope of this article.

In spite of its numerous advantageous features, Wynn’s epsilon algorithm (3.1) is not suited for our purposes. If the input data are the partial sums (1.4) of the (formal) power series (1.3), the accuracy-through-order relationship (1.6) of Padé approximants in combination with (3.2) implies that the elements of the epsilon table with even subscripts can be expressed as

$$\varepsilon_{2k}^{(n)} = f_{n+2k}(z) + g_{2k}^{(n)} z^{n+2k+1} + O(z^{n+2k+2}), \quad z \rightarrow 0. \tag{3.3}$$

The constant $g_{2k}^{(n)}$ is the prediction made for the coefficient γ_{n+2k+1} , which is the first coefficient of the power series (1.3) not used for the computation of $\varepsilon_{2k}^{(n)}$.

If we compute $\varepsilon_2^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, and $f_{n+2}(z)$, we obtain because of $\mathcal{A}_1^{(n)} = \varepsilon_2^{(n)}$ the same expressions as in the last section. Thus, we obtain a result which does not seem to be in agreement with the accuracy-through-order relationship (3.3):

$$\varepsilon_2^{(n)} = f_{n+1}(z) + \frac{\gamma_{n+1}\gamma_{n+2}z^{n+2}}{\gamma_{n+1} - \gamma_{n+2}z}. \tag{3.4}$$

Of course, the missing term $\gamma_{n+2}z^{n+2}$ can easily be extracted from the rational expression on the right-hand side. We only have to use $1/(1 - y) = 1 + y/(1 - y)$ with $y = \gamma_{n+2}z/\gamma_{n+1}$ to obtain as in the case of Aitken’s iterated Δ^2 algorithm an expression with the desired features:

$$\varepsilon_2^{(n)} = f_{n+2}(z) + \frac{[\gamma_{n+2}]^2 z^{n+3}}{\gamma_{n+1} - \gamma_{n+2}z}. \tag{3.5}$$

This example shows that the accuracy-through-order relationship (1.6) of Padé approximants is by no means immediately obvious from the epsilon algorithm (3.1). A further complication is that the epsilon algorithm involves the elements $\varepsilon_{2k+1}^{(n)}$ with odd subscripts. These are only auxiliary quantities which diverge if the whole process converges. Nevertheless, they make it difficult to obtain order estimates and to reformulate the epsilon algorithm in such a way that it automatically produces suitable expressions for $\varepsilon_{2k}^{(n)}$ of the type of (3.5).

The starting point for the construction of an alternative recursive scheme, which would be suited for our purposes, is Wynn’s cross rule [118, Eq. (13)]:

$$\{\varepsilon_{2k+2}^{(n)} - \varepsilon_{2k}^{(n+1)}\}^{-1} + \{\varepsilon_{2k-2}^{(n+2)} - \varepsilon_{2k}^{(n+1)}\}^{-1} = \{\varepsilon_{2k}^{(n)} - \varepsilon_{2k}^{(n+1)}\}^{-1} + \{\varepsilon_{2k}^{(n+2)} - \varepsilon_{2k}^{(n+1)}\}^{-1}. \tag{3.6}$$

This expression permits the recursive computation of the elements $\varepsilon_{2k}^{(n)}$ with even subscripts without having to compute the auxiliary quantities $\varepsilon_{2k+1}^{(n)}$ with odd subscripts. The price, one has to pay, is that the cross-rule (3.6) has a more complicated structure than the extremely simple epsilon algorithm (3.1).

A further complication is that for $k = 0$ the undefined element $\varepsilon_{-2}^{(n)}$ occurs in (3.6). However, we obtain results that are consistent with Wynn’s epsilon algorithm (3.1) if we set $\varepsilon_{-2}^{(n)} = \infty$.

Hence, instead of the epsilon algorithm (3.1), we can also use the following recursive scheme:

$$\varepsilon_{-2}^{(n)} = \infty, \quad \varepsilon_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{3.7a}$$

$$\varepsilon_{2k+2}^{(n)} = \varepsilon_{2k}^{(n+1)} + \frac{1}{1/\Delta\varepsilon_{2k}^{(n+1)} - 1/\Delta\varepsilon_{2k}^{(n)} + 1/(\varepsilon_{2k}^{(n+1)} - \varepsilon_{2k-2}^{(n+2)}), \quad k, n \in \mathbb{N}_0. \tag{3.7b}$$

For our purposes, this recursive scheme is an improvement over the epsilon algorithm (3.1) since it does not contain the elements $\varepsilon_{2k+1}^{(n)}$ with odd subscripts. Nevertheless, it is not yet what we need. The use of (3.7) for the computation of $\varepsilon_2^{(n)}$ would produce (3.4) but not (3.5). Fortunately, (3.7) can easily be modified to yield a recursive scheme having the desired features:

$$\varepsilon_{-2}^{(n)} = \infty, \quad \varepsilon_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{3.8a}$$

$$\varepsilon_{2k+2}^{(n)} = \varepsilon_{2k}^{(n+2)} + \frac{\Delta\varepsilon_{2k}^{(n+1)}/\Delta\varepsilon_{2k}^{(n)} - \Delta\varepsilon_{2k}^{(n+1)}/(\varepsilon_{2k}^{(n+1)} - \varepsilon_{2k-2}^{(n+2)})}{1/\Delta\varepsilon_{2k}^{(n+1)} - 1/\Delta\varepsilon_{2k}^{(n)} + 1/(\varepsilon_{2k}^{(n+1)} - \varepsilon_{2k-2}^{(n+2)}), \quad k, n \in \mathbb{N}_0. \tag{3.8b}$$

If we use (3.8) for the computation of $\varepsilon_2^{(n)}$, we obtain (3.5).

Next, we use in (3.8) the partial sums (1.4) of the (formal) power series (1.3) in the form of (2.12). This yields

$$\varepsilon_{2k}^{(n)} = f(z) + z^{n+2k+1}r_{2k}^{(n)}(z), \quad k, n \in \mathbb{N}_0. \tag{3.9}$$

The quantities $r_{2k}^{(n)}(z)$ can be computed with the help of the following recursive scheme which is a direct consequence of the recursive scheme (3.8) for $\varepsilon_{2k}^{(n)}$:

$$r_0^{(n)}(z) = - \sum_{v=0}^{\infty} \gamma_{n+v+1} z^v = \frac{f_n(z) - f(z)}{z^{n+1}}, \quad n \in \mathbb{N}_0, \tag{3.10a}$$

$$r_2^{(n)}(z) = r_0^{(n+2)}(z) + \frac{\delta r_0^{(n+1)}(z)/\delta r_0^{(n)}(z)}{1/\delta r_0^{(n+1)}(z) - z/\delta r_0^{(n)}(z)}, \quad n \in \mathbb{N}_0, \tag{3.10b}$$

$$r_{2k+2}^{(n)}(z) = r_{2k}^{(n+2)}(z) + \frac{\delta r_{2k}^{(n+1)}(z)/\delta r_{2k}^{(n)}(z) - \delta r_{2k}^{(n+1)}(z)/(zr_{2k}^{(n+1)}(z) - r_{2k-2}^{(n+2)}(z))}{1/\delta r_{2k}^{(n+1)}(z) - z/\delta r_{2k}^{(n)}(z) + z/(zr_{2k}^{(n+1)}(z) - r_{2k-2}^{(n+2)}(z))}, \quad k, n \in \mathbb{N}_0. \tag{3.10c}$$

Here, $\delta r_{2k}^{(n)}(z)$ is defined by (2.15). It should be noted that (3.10b) follows from (3.10c) if we define $r_{-2}^{(n)}(z) = \infty$.

Similar to the analogous accuracy-through-order relationship (2.13) for Aitken’s iterated Δ^2 process, (3.9) has the right structure to serve as an accuracy-through-order relationship for Wynn’s epsilon algorithm. Thus, it seems that we have accomplished our aim. However, we are faced with

the same complications as in the case of (2.13). If $z^{n+2k+1}r_{2k}^{(n)}(z)$ in (3.9) is to be of order $O(z^{n+2k+1})$ as $z \rightarrow 0$, then the z -independent part $c_{2k}^{(n)}$ of $r_{2k}^{(n)}(z)$ defined by

$$r_{2k}^{(n)}(z) = c_{2k}^{(n)} + O(z), \quad z \rightarrow 0 \tag{3.11}$$

has to satisfy

$$c_{2k}^{(n)} \neq 0, \quad k, n \in \mathbb{N}_0. \tag{3.12}$$

If this condition is satisfied, we can be sure that (3.9) is indeed the accuracy-through-order relationship we have been looking for.

As in the case of Aitken’s iterated Δ^2 process, it is by no means obvious whether and how it can be proven that a given power series gives rise to truncation errors $r_{2k}^{(n)}(z)$ satisfying (3.11) and (3.12). Fortunately, it can easily be checked *numerically* whether a given (formal) power series leads to truncations errors whose z -independent parts are nonzero. If we set $z = 0$ in (3.10) and use (3.11), we obtain the following recursive scheme:

$$c_0^{(n)} = -\gamma_{n+1}, \quad n \in \mathbb{N}_0, \tag{3.13a}$$

$$c_2^{(n)} = c_0^{(n+2)} - \frac{[c_0^{(n+1)}]^2}{c_0^{(n)}}, \quad n \in \mathbb{N}_0, \tag{3.13b}$$

$$c_{2k+2}^{(n)} = c_{2k}^{(n+2)} - \frac{[c_{2k}^{(n+1)}]^2}{c_{2k}^{(n)}} + \frac{[c_{2k}^{(n+1)}]^2}{c_{2k-2}^{(n+2)}}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{3.13c}$$

If we define $c_{-2}^{(n)} = \infty$, then (3.13b) follows from (3.13c).

Let us now assume that we know for a given (formal) power series that the z -independent parts $c_{2k}^{(n)}$ of the truncation errors $r_{2k}^{(n)}(z)$ in (3.9) are nonzero — either from a mathematical proof or from a brute force calculation using (3.13). Then, (3.9) is indeed the accuracy-through-order relationship we have been looking for. This implies that $\varepsilon_{2k}^{(n)}$ can be expressed as follows:

$$\varepsilon_{2k}^{(n)} = f_{n+2k}(z) + z^{n+2k+1}\varphi_{2k}^{(n)}(z). \tag{3.14}$$

If we use this ansatz in (3.8), we obtain the following recursive scheme:

$$\varphi_0^{(n)}(z) = 0, \quad n \in \mathbb{N}_0, \tag{3.15a}$$

$$\varphi_2^{(n)}(z) = \frac{[\gamma_{n+2}]^2}{\gamma_{n+1} - \gamma_{n+2}z}, \quad n \in \mathbb{N}_0, \tag{3.15b}$$

$$\varphi_{2k+2}^{(n)}(z) = \varphi_{2k}^{(n+2)}(z) + \frac{\alpha_{2k+2}^{(n)}(z)}{\beta_{2k+2}^{(n)}(z)}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0, \tag{3.15c}$$

$$\alpha_{2k+2}^{(n)}(z) = \frac{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)}{\gamma_{n+2k+1} + \delta\varphi_{2k}^{(n)}(z)} - \frac{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)}{\gamma_{n+2k+1} + z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k-2}^{(n+2)}(z)}, \tag{3.15d}$$

$$\begin{aligned} \beta_{2k+2}^{(n)}(z) &= \frac{1}{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)} - \frac{z}{\gamma_{n+2k+1} + \delta\varphi_{2k}^{(n)}(z)} \\ &+ \frac{z}{\gamma_{n+2k+1} + z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k-2}^{(n+2)}(z)}. \end{aligned} \tag{3.15e}$$

Here, $\delta\varphi_{2k}^{(n)}(z)$ is defined by (2.15). Moreover, we could also define $\varphi_{-2}^{(n)}(z) = \infty$. Then, (3.15b) would follow from (3.15c).

A comparison of (3.3) and (3.14) yields

$$\varphi_{2k}^{(n)}(z) = g_{2k}^{(n)} + O(z), \quad z \rightarrow 0. \tag{3.16}$$

Consequently, the z -independent part $g_{2k}^{(n)}$ of $\varphi_{2k}^{(n)}(z)$ is the prediction for the first coefficient γ_{n+2k+1} not used for the computation of $\varepsilon_{2k}^{(n)}$.

If we set $z = 0$ in the recursive scheme (3.15) and use (3.16), we obtain the following recursive scheme for the predictions $g_{2k}^{(n)}$:

$$g_0^{(n)} = 0, \quad n \in \mathbb{N}_0, \tag{3.17a}$$

$$g_2^{(n)} = \frac{[\gamma_{n+2}]^2}{\gamma_{n+1}}, \quad n \in \mathbb{N}_0, \tag{3.17b}$$

$$g_{2k+2}^{(n)} = g_{2k}^{(n+2)} + \frac{[\gamma_{n+2k+2} - g_{2k}^{(n+1)}]^2}{\gamma_{n+2k+1} - g_{2k}^{(n)}} - \frac{[\gamma_{n+2k+2} - g_{2k}^{(n+1)}]^2}{\gamma_{n+2k+1} - g_{2k-2}^{(n+2)}}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{3.17c}$$

If we define $g_{-2}^{(n)} = \infty$, then (3.17b) follows from (3.17a) and (3.17c).

The z -independent parts $c_{2k}^{(n)}$ of $r_{2k}^{(n)}(z)$ and $g_{2k}^{(n)}$ of $\varphi_{2k}^{(n)}(z)$, respectively, are connected. A comparison of (3.9), (3.11), (3.14), and (3.16) yields

$$g_{2k}^{(n)} = c_{2k}^{(n)} + \gamma_{n+2k+1}. \tag{3.18}$$

Concerning the choice of the approximation to the limit, we proceed in the case of the epsilon algorithm just like in the case of Aitken’s iterated Δ^2 process and compute a new approximation to the limit after the computation of each new partial sum. Thus, if the index m of the last partial sum $f_m(z)$ is even, $m = 2\mu$, we use as approximation to the limit $f(z)$ the transformation

$$\{f_0(z), f_1(z), \dots, f_{2\mu}(z)\} \mapsto \varepsilon_{2\mu}^{(0)} \tag{3.19}$$

and if m is odd, $m = 2\mu + 1$, we use the transformation

$$\{f_1(z), f_2(z), \dots, f_{2\mu+1}(z)\} \mapsto \varepsilon_{2\mu}^{(1)}. \tag{3.20}$$

These two relationships can be combined into a single equation, yielding [95, Eq. (4.3–6)]

$$\{f_{m-2\lfloor m/2\rfloor}(z), f_{m-2\lfloor m/2\rfloor+1}(z), \dots, f_m(z)\} \mapsto \varepsilon_{2\lfloor m/2\rfloor}^{(m-2\lfloor m/2\rfloor)}, \quad m \in \mathbb{N}_0. \tag{3.21}$$

4. The iteration of Brezinski’s theta algorithm

Brezinski’s theta algorithm is the following recursive scheme [13]:

$$\vartheta_{-1}^{(n)} = 0, \quad \vartheta_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{4.1a}$$

$$\vartheta_{2k+1}^{(n)} = \vartheta_{2k-1}^{(n+1)} + 1/[\Delta\vartheta_{2k}^{(n)}], \quad k, n \in \mathbb{N}_0, \tag{4.1b}$$

$$\vartheta_{2k+2}^{(n)} = \vartheta_{2k}^{(n+1)} + \frac{[\Delta\vartheta_{2k}^{(n+1)}][\Delta\vartheta_{2k+1}^{(n+1)}]}{\Delta^2\vartheta_{2k+1}^{(n)}}, \quad k, n \in \mathbb{N}_0. \tag{4.1c}$$

As in the case of Wynn’s epsilon algorithm (3.1), only the elements $\vartheta_{2k}^{(n)}$ with even subscripts provide approximations to the (generalized) limit of the sequence to be transformed. The elements $\vartheta_{2k+1}^{(n)}$ with odd subscripts are only auxiliary quantities which diverge if the whole process converges.

The theta algorithm was derived from Wynn’s epsilon algorithm (3.1) with the intention of overcoming the inability of the epsilon algorithm to accelerate logarithmic convergence. In that respect, the theta algorithm was a great success. Extensive numerical studies of Smith and Ford [87,88] showed that the theta algorithm is not only very powerful, but also much more versatile than the epsilon algorithm. Like the epsilon algorithm, it is an efficient accelerator for linear convergence and it is also able to sum many divergent series. However, it is also able to accelerate the convergence of many logarithmically convergent sequences and series.

As for example discussed in [97], new sequence transformations can be constructed by iterating explicit expressions for sequence transformations with low transformation orders. The best known example of such an iterated sequence transformation is probably Aitken’s iterated Δ^2 process (2.4) which is obtained by iterating Aitken’s Δ^2 formula (2.2).

The same approach is also possible in the case of the theta algorithm. A suitable closed-form expression, which may be iterated, is [95, Eq. (10.3–1)]

$$\vartheta_2^{(n)} = s_{n+1} - \frac{[\Delta s_n][\Delta s_{n+1}][\Delta^2 s_{n+1}]}{[\Delta s_{n+2}][\Delta^2 s_n] - [\Delta s_n][\Delta^2 s_{n+1}]}, \quad n \in \mathbb{N}_0. \tag{4.2}$$

The iteration of this expression yields the following nonlinear recursive scheme [95, Eq. (10.3–6)]:

$$\mathcal{J}_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{4.3a}$$

$$\mathcal{J}_{k+1}^{(n)} = \mathcal{J}_k^{(n+1)} - \frac{[\Delta \mathcal{J}_k^{(n)}][\Delta \mathcal{J}_k^{(n+1)}][\Delta^2 \mathcal{J}_k^{(n+1)}]}{[\Delta \mathcal{J}_k^{(n+2)}][\Delta^2 \mathcal{J}_k^{(n)}] - [\Delta \mathcal{J}_k^{(n)}][\Delta^2 \mathcal{J}_k^{(n+1)}]}, \quad k, n \in \mathbb{N}_0. \tag{4.3b}$$

In convergence acceleration and summation processes, the iterated transformation $\mathcal{J}_k^{(n)}$ has similar properties as the theta algorithm from which it was derived: They are both very powerful as well as very versatile. $\mathcal{J}_k^{(n)}$ is not only an effective accelerator for linear convergence as well as able to sum divergent series, but it is also able to accelerate the convergence of many logarithmically convergent sequences and series [11,74–77,95,97,100].

In spite of all these similarities, the iterated transformation $\mathcal{J}_k^{(n)}$ has one undeniable advantage over the theta algorithm, which ultimately explains why in this article only $\mathcal{J}_k^{(n)}$ is studied, but not the theta algorithm: The recursive scheme (4.3) for $\mathcal{J}_k^{(n)}$ is slightly less complicated than the recursive scheme (4.1) for the theta algorithm. On p. 282 of Weniger [95] it was emphasized that a replacement of (4.1b) by the simpler recursion

$$\vartheta_{2k+1}^{(n)} = 1/[\Delta \vartheta_{2k}^{(n)}], \quad k, n \in \mathbb{N}_0 \tag{4.4}$$

would lead to a modified theta algorithm which satisfies $\vartheta_{2k}^{(n)} = \mathcal{J}_k^{(n)}$.

It is a direct consequence of the recursive scheme (4.3) that $3k + 1$ sequence elements $s_n, s_{n+1}, \dots, s_{n+3k}$ are needed for the computation of $\mathcal{J}_k^{(n)}$. Thus, we now choose as input data the partial sums (1.4) of the (formal) power series (1.3) according to $s_n = f_n(z)$, and conjecture that all coefficients $\gamma_0, \gamma_1, \dots, \gamma_{n+3k}$, which were used for the construction of $\mathcal{J}_k^{(n)}$, are exactly reproduced by a Taylor expansion. This means that we have to look for an accuracy-through-order relationship of the following kind:

$$f(z) - \mathcal{J}_k^{(n)} = O(z^{n+3k+1}), \quad z \rightarrow 0. \tag{4.5}$$

Such an accuracy-through-order relationship would imply that $\mathcal{J}_k^{(n)}$ can be expressed as follows:

$$\mathcal{J}_k^{(n)} = f_{n+3k}(z) + \mathcal{G}_k^{(n)} z^{n+3k+1} + O(z^{n+3k+2}), \quad z \rightarrow 0. \tag{4.6}$$

The constant $\mathcal{G}_k^{(n)}$ is the prediction made for the coefficient γ_{n+3k+1} , which is the first coefficient of the power series (1.3) not used for the computation of $\mathcal{J}_k^{(n)}$.

Unfortunately, the recursive scheme (4.3) is not suited for our purposes. This can be shown by computing $\mathcal{J}_1^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, $f_{n+2}(z)$, and $f_{n+3}(z)$:

$$\mathcal{J}_1^{(n)} = f_{n+1}(z) - \frac{\gamma_{n+1}\gamma_{n+2}[\gamma_{n+3}z - \gamma_{n+2}]z^{n+2}}{\gamma_{n+3}z[\gamma_{n+2}z - \gamma_{n+1}] - \gamma_{n+1}[\gamma_{n+3}z - \gamma_{n+2}]} \tag{4.7}$$

Superficially, it looks as if the accuracy-through-order relationship (4.5) is not satisfied by $\mathcal{J}_1^{(n)}$. However, the rational expression on the right-hand side contains the missing terms $\gamma_{n+2}z^{n+2}$ and $\gamma_{n+3}z^{n+3}$, as shown by the Taylor expansion

$$\begin{aligned} & - \frac{\gamma_{n+1}\gamma_{n+2}[\gamma_{n+3}z - \gamma_{n+2}]z^{n+2}}{\gamma_{n+3}z[\gamma_{n+2}z - \gamma_{n+1}] - \gamma_{n+1}[\gamma_{n+3}z - \gamma_{n+2}]} \\ & = \gamma_{n+2}z^{n+2} + \gamma_{n+3}z^{n+3} - \frac{\gamma_{n+3}\{[\gamma_{n+2}]^2 - 2\gamma_{n+1}\gamma_{n+3}\}z^{n+4}}{\gamma_{n+1}\gamma_{n+2}} + O(z^{n+5}). \end{aligned} \tag{4.8}$$

Thus, an expression, which is in agreement with (4.6), can be obtained easily in the case of the simplest transform $\mathcal{J}_1^{(n)}$. Moreover, the Taylor expansion (4.8) shows that $\mathcal{J}_1^{(n)}$ makes the prediction

$$\mathcal{G}_1^{(n)} = - \frac{\gamma_{n+3}\{[\gamma_{n+2}]^2 - 2\gamma_{n+1}\gamma_{n+3}\}}{\gamma_{n+1}\gamma_{n+2}} \tag{4.9}$$

for the first series coefficient γ_{n+4} not used for the computation of $\mathcal{J}_1^{(n)}$. Of course, by including additional terms in the Taylor expansion (4.8) further predictions on series coefficients with higher indices can be made.

However, in the case of more complicated transforms $\mathcal{J}_k^{(n)}$ with $k > 1$ it by no means is obvious whether and how an expression, which is in agreement with (4.6), can be constructed. Consequently, it is certainly a good idea to replace the recursive scheme (4.3) by an alternative recursive scheme, which directly leads to appropriate expressions for $\mathcal{J}_k^{(n)}$ with $k > 1$.

Many different expressions for $\vartheta_2^{(n)}$ in terms of s_n, s_{n+1}, s_{n+2} , and s_{n+3} are known [95, Section 10.4]. For our purposes the appropriate expression is

$$\vartheta_2^{(n)} = s_{n+3} - \frac{[\Delta s_{n+2}]\{[\Delta s_{n+2}][\Delta^2 s_n] + [\Delta s_{n+1}]^2 - [\Delta s_{n+2}][\Delta s_n]\}}{[\Delta s_{n+2}][\Delta^2 s_n] - [\Delta s_n][\Delta^2 s_{n+1}]} \tag{4.10}$$

Just like (4.2), this expression can be iterated and yields

$$\mathcal{J}_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \tag{4.11a}$$

$$\mathcal{J}_{k+1}^{(n)} = \mathcal{J}_k^{(n+3)} - \frac{A_{k+1}^{(n)}}{B_{k+1}^{(n)}}, \quad k, n \in \mathbb{N}_0, \tag{4.11b}$$

$$A_{k+1}^{(n)} = [\Delta \mathcal{J}_k^{(n+2)}]\{[\Delta \mathcal{J}_k^{(n+2)}][\Delta^2 \mathcal{J}_k^{(n)}] + [\Delta \mathcal{J}_k^{(n+1)}]^2 - [\Delta \mathcal{J}_k^{(n)}][\Delta \mathcal{J}_k^{(n+2)}]\}, \tag{4.11c}$$

$$B_{k+1}^{(n)} = [\Delta \mathcal{J}_k^{(n+2)}][\Delta^2 \mathcal{J}_k^{(n)}] - [\Delta \mathcal{J}_k^{(n)}][\Delta^2 \mathcal{J}_k^{(n+1)}]. \tag{4.11d}$$

If we now use either (4.10) or (4.11) to compute $\mathcal{J}_1^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, $f_{n+2}(z)$, and $f_{n+3}(z)$, we obtain the following expression which obviously possesses the desired features:

$$\mathcal{J}_1^{(n)} = f_{n+3}(z) - \frac{\gamma_{n+3}\{\gamma_{n+3}[\gamma_{n+2}z - \gamma_{n+1}] + [\gamma_{n+2}]^2 - \gamma_{n+1}\gamma_{n+3}\}z^{n+4}}{\gamma_{n+3}z[\gamma_{n+2}z - \gamma_{n+1}] - \gamma_{n+1}[\gamma_{n+3}z - \gamma_{n+2}]} \tag{4.12}$$

Next, we use in (4.11) the partial sums (1.4) of the (formal) power series (1.3) in the form of (2.12). This yields

$$\mathcal{R}_k^{(n)} = f(z) + z^{n+3k+1}\mathcal{R}_k^{(n)}(z), \quad k, n \in \mathbb{N}_0. \tag{4.13}$$

The quantities $\mathcal{R}_k^{(n)}(z)$ can be computed with the help of the following recursive scheme which is a direct consequence of the recursive scheme (4.11) for $\mathcal{J}_k^{(n)}$:

$$\mathcal{R}_0^{(n)}(z) = - \sum_{v=0}^{\infty} \gamma_{n+v+1}z^v = \frac{f_n(z) - f(z)}{z^{n+1}}, \quad n \in \mathbb{N}_0, \tag{4.14a}$$

$$\mathcal{R}_{k+1}^{(n)}(z) = \mathcal{R}_k^{(n+3)}(z) - \frac{\mathcal{N}_{k+1}^{(n)}(z)}{\mathcal{D}_{k+1}^{(n)}(z)}, \quad k, n \in \mathbb{N}_0, \tag{4.14b}$$

$$\mathcal{N}_{k+1}^{(n)}(z) = [\delta\mathcal{R}_k^{(n+2)}(z)]\{[\delta\mathcal{R}_k^{(n+2)}(z)][\delta^2\mathcal{R}_k^{(n)}(z)] + [\delta\mathcal{R}_k^{(n+1)}(z)]^2 - [\delta\mathcal{R}_k^{(n)}(z)][\delta\mathcal{R}_k^{(n+2)}(z)]\}, \tag{4.14c}$$

$$\mathcal{D}_{k+1}^{(n)}(z) = z[\delta\mathcal{R}_k^{(n+2)}(z)][\delta^2\mathcal{R}_k^{(n)}(z)] - [\delta\mathcal{R}_k^{(n)}(z)][\delta^2\mathcal{R}_k^{(n+1)}(z)]. \tag{4.14d}$$

Here, $\delta\mathcal{R}_k^{(n+2)}(z)$ and $\delta^2\mathcal{R}_k^{(n+2)}(z)$ are defined by (2.15).

Similar to the analogous accuracy-through-order relationships (2.13) and (3.9) for Aitken’s iterated Δ^2 process and the epsilon algorithm, respectively, (4.13) has the right structure to serve as an accuracy-through-order relationship for the iterated theta algorithm. Thus, it seems that we have accomplished our aim. However, we are faced with the same complications as in the case of (2.13) and (3.9). If $z^{n+3k+1}\mathcal{R}_{2k}^{(n)}(z)$ in (4.13) is to be of order $O(z^{n+3k+1})$ as $z \rightarrow 0$, then the z -independent part $\mathcal{C}_k^{(n)}$ of $\mathcal{R}_k^{(n)}(z)$ defined by

$$\mathcal{R}_k^{(n)}(z) = \mathcal{C}_k^{(n)} + O(z), \quad z \rightarrow 0, \tag{4.15}$$

has to satisfy

$$\mathcal{C}_k^{(n)} \neq 0, \quad k, n \in \mathbb{N}_0. \tag{4.16}$$

If this condition is satisfied, then it is guaranteed that (4.13) is indeed the accuracy-through-order relationship we have been looking for.

As in the case of Aitken’s iterated Δ^2 process or the epsilon algorithm, it is by no means obvious whether and how it can be proven that a given power series gives rise to truncation errors $\mathcal{R}_k^{(n)}(z)$ satisfying (4.15) and (4.16). Fortunately, it can easily be checked *numerically* whether a given (formal) power series leads to truncations errors whose z -independent parts are nonzero. If we set

$z = 0$ in (4.14) and use (4.15), we obtain the following recursive scheme:

$$\mathcal{C}_0^{(n)} = -\gamma_{n+1}, \quad n \in \mathbb{N}_0, \tag{4.17a}$$

$$\mathcal{C}_{k+1}^{(n)} = \mathcal{C}_k^{(n+3)} - \frac{\mathcal{C}_k^{(n+2)} \{2\mathcal{C}_k^{(n)}\mathcal{C}_k^{(n+2)} - [\mathcal{C}_k^{(n+1)}]^2\}}{\mathcal{C}_k^{(n)}\mathcal{C}_k^{(n+1)}}, \quad k, n \in \mathbb{N}_0. \tag{4.17b}$$

Let us now assume that we know for a given (formal) power series that the z -independent parts $\mathcal{C}_k^{(n)}$ of the truncation errors $\mathcal{R}_k^{(n)}(z)$ in (4.13) are nonzero — either from a mathematical proof or from a brute force calculation using (4.17). Then, (4.13) is indeed the accuracy-through-order relationship we have been looking for. This implies that $\mathcal{F}_k^{(n)}$ can be expressed as follows:

$$\mathcal{F}_k^{(n)} = f_{n+3k}(z) + z^{n+3k+1} \Psi_k^{(n)}(z), \quad k, n \in \mathbb{N}_0. \tag{4.18}$$

If we use this ansatz in (4.11), we obtain the following recursive scheme:

$$\Psi_0^{(n)}(z) = 0, \quad n \in \mathbb{N}_0, \tag{4.19a}$$

$$\Psi_1^{(n)}(z) = -\frac{\gamma_{n+3} \{ \gamma_{n+3} [\gamma_{n+2} z - \gamma_{n+1}] + [\gamma_{n+2}]^2 - \gamma_{n+1} \gamma_{n+3} \}}{\gamma_{n+3} [\gamma_{n+2} z - \gamma_{n+1}] - \gamma_{n+1} [\gamma_{n+3} z - \gamma_{n+2}]}, \quad n \in \mathbb{N}_0, \tag{4.19b}$$

$$\Psi_{k+1}^{(n)}(z) = \Psi_k^{(n+3)}(z) - \frac{N_{k+1}^{(n)}(z)}{D_{k+1}^{(n)}(z)}, \quad k, n \in \mathbb{N}_0, \tag{4.19c}$$

$$N_{k+1}^{(n)}(z) = [\gamma_{n+3k+3} + \delta \Psi_k^{(n+2)}(z)] \{ [\gamma_{n+3k+3} + \delta \Psi_k^{(n+2)}(z)] [\gamma_{n+3k+2} z - \gamma_{n+3k+1} + \delta^2 \Psi_k^{(n)}(z)] + [\gamma_{n+3k+2} + \delta \Psi_k^{(n+1)}(z)]^2 - [\gamma_{n+3k+1} + \delta \Psi_k^{(n)}(z)] [\gamma_{n+3k+3} + \delta \Psi_k^{(n+2)}(z)] \}, \tag{4.19d}$$

$$D_{k+1}^{(n)}(z) = [\gamma_{n+3k+3} + \delta \Psi_k^{(n+2)}(z)] [\gamma_{n+3k+2} z - \gamma_{n+3k+1} + \delta^2 \Psi_k^{(n)}(z)] - [\gamma_{n+3k+1} + \delta \Psi_k^{(n)}(z)] [\gamma_{n+3k+3} z - \gamma_{n+3k+2} + \delta^2 \Psi_k^{(n+1)}(z)]. \tag{4.19e}$$

Here, $\delta \Psi_k^{(n+2)}(z)$ and $\delta^2 \Psi_k^{(n+2)}(z)$ are defined by (2.15).

A comparison of (4.6) and (4.18) yields

$$\Psi_k^{(n)}(z) = \mathcal{G}_k^{(n)} + O(z), \quad z \rightarrow 0. \tag{4.20}$$

Consequently, the z -independent part $\mathcal{G}_k^{(n)}$ of $\Psi_k^{(n)}(z)$ is the prediction for the first coefficient γ_{n+3k+1} not used for the computation of $\mathcal{F}_k^{(n)}$.

If we set $z = 0$ in the recursive scheme (4.19) and use (4.20), we obtain the following recursive scheme for the predictions $\mathcal{G}_k^{(n)}$:

$$\mathcal{G}_0^{(n)} = 0, \quad n \in \mathbb{N}_0, \tag{4.21a}$$

$$\mathcal{G}_1^{(n)} = -\frac{\gamma_{n+3} \{ [\gamma_{n+2}]^2 - 2\gamma_{n+1} \gamma_{n+3} \}}{\gamma_{n+1} \gamma_{n+2}}, \quad n \in \mathbb{N}_0, \tag{4.21b}$$

$$\mathcal{G}_{k+1}^{(n)} = \mathcal{G}_k^{(n+3)} - \frac{F_{k+1}^{(n)}}{H_{k+1}^{(n)}}, \quad k, n \in \mathbb{N}_0, \tag{4.21c}$$

$$F_{k+1}^{(n)} = [\gamma_{n+3k+3} - \mathcal{G}_k^{(n+2)}] \{ [\gamma_{n+3k+2} - \mathcal{G}_k^{(n+1)}]^2 - 2[\gamma_{n+3k+1} - \mathcal{G}_k^{(n)}][\gamma_{n+3k+3} - \mathcal{G}_k^{(n+2)}] \}, \tag{4.21d}$$

$$H_{k+1}^{(n)} = [\gamma_{n+3k+1} - \mathcal{G}_k^{(n)}][\gamma_{n+3k+2} - \mathcal{G}_k^{(n+1)}]. \tag{4.21e}$$

The z -independent parts $\mathcal{C}_k^{(n)}$ of $\mathcal{R}_k^{(n)}(z)$ and $\mathcal{G}_k^{(n)}$ of $\Psi_k^{(n)}(z)$, respectively, are connected. A comparison of (4.13), (4.15), (4.18), and (4.20) yields

$$\mathcal{G}_k^{(n)} = \mathcal{C}_k^{(n)} + \gamma_{n+3k+1}. \tag{4.22}$$

As in the case of Aitken’s iterated Δ^2 process or Wynn’s epsilon algorithm, a new approximation to the limit will be computed after the computation of each new partial sum. Thus, if the index m of the last partial sum $f_m(z)$ is a multiple of 3, $m = 3\mu$, we use as approximation to the limit $f(z)$ the transformation

$$\{f_0(z), f_1(z), \dots, f_{3\mu}(z)\} \mapsto J_\mu^{(0)}, \tag{4.23}$$

if we have $m = 3\mu + 1$, we use the transformation

$$\{f_1(z), f_2(z), \dots, f_{3\mu+1}(z)\} \mapsto \mathcal{J}_\mu^{(1)}, \tag{4.24}$$

and if we have $m = 3\mu + 2$, we use the transformation

$$\{f_2(z), f_3(z), \dots, f_{3\mu+2}(z)\} \mapsto \mathcal{J}_\mu^{(2)}, \tag{4.25}$$

These three relationships can be combined into a single equation, yielding [95, Eq. (10.4-7)]

$$\{f_{m-3\lfloor m/3\rfloor}(z), f_{m-3\lfloor m/3\rfloor+1}(z), \dots, f_m(z)\} \mapsto \mathcal{J}_{\lfloor m/3\rfloor}^{(m-3\lfloor m/3\rfloor)}, \quad m \in \mathbb{N}_0. \tag{4.26}$$

5. Applications

In this article, two principally different kinds of results were derived. The first group of results — the accuracy-through-order relationships (2.13), (3.9), and (4.13) and the corresponding recursive schemes (2.14), (3.9), and (4.14) — defines the transformation error terms $z^{n+2k+1}R_k^{(n)}(z)$, $z^{n+2k+1}r_{2k}^{(n)}(z)$, and $z^{n+3k+1}\mathcal{R}_k^{(n)}(z)$. These quantities describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\mathcal{E}_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the function $f(z)$ which is to be approximated. Obviously, the transformation error terms must vanish if the transformation process converges.

The second group of results — (2.19), (3.14), and (4.18) and the corresponding recursive schemes (2.20), (3.15), and (4.19) — defines the terms $z^{n+2k+1}\Phi_k^{(n)}(z)$, $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$, and $z^{n+3k+1}\Psi_k^{(n)}(z)$. These quantities describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\mathcal{E}_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the partial sums $f_{n+2k}(z)$ and $f_{n+3k}(z)$, respectively, from which they were constructed. Hence, the first group of results essentially describes what is still missing in the transformation process, whereas the second group describes what was gained by constructing rational expressions from the partial sums.

The recursive schemes (2.14), (3.9), and (4.14) of the first group use as input data the remainder terms

$$\frac{f_n(z) - f(z)}{z^{n+1}} = - \sum_{v=0}^{\infty} \gamma_{n+v+1} z^v. \tag{5.1}$$

In most practically relevant convergence acceleration and summation problems, only a finite number of series coefficients γ_v are known. Consequently, the remainder terms (5.1) are usually not known

explicitly, which means that the immediate practical usefulness of the first group of results is quite limited. Nevertheless, these results are of interest because they can be used to study the convergence of the sequence transformations of this article for model problems.

As an example, let us consider the following series expansion for the logarithm

$$\frac{\ln(1+z)}{z} = {}_2F_1(1, 1; 2; -z) = \sum_{m=0}^{\infty} \frac{(-z)^m}{m+1}, \tag{5.2}$$

which converges for all $z \in \mathbb{C}$ with $|z| < 1$. The logarithm possesses the integral representation

$$\frac{\ln(1+z)}{z} = \int_0^1 \frac{dt}{1+zt}, \tag{5.3}$$

which shows that $\ln(1+z)/z$ is a Stieltjes function and that the hypergeometric series on the right-hand side of (5.2) is the corresponding Stieltjes series (a detailed treatment of Stieltjes functions and Stieltjes series can for example be found in Section 5 of Baker and Graves-Morris [8]). Consequently, $\ln(1+z)/z$ possesses the following representation as a partial sum plus an explicit remainder which is given by a Stieltjes integral (compare for example Eq. (13.1-5) of Weniger [95]):

$$\frac{\ln(1+z)}{z} = \sum_{m=0}^n \frac{(-z)^m}{m+1} + (-z)^{n+1} \int_0^1 \frac{t^{n+1} dt}{1+zt}, \quad n \in \mathbb{N}_0. \tag{5.4}$$

For $|z| < 1$, the denominator of the remainder integral on the right-hand side can be expanded. Interchanging summation and integration then yields

$$(-1)^{n+1} \int_0^1 \frac{t^{n+1} dt}{1+zt} = \sum_{m=0}^{\infty} \frac{(-1)^{n+m+1} z^m}{n+m+2}. \tag{5.5}$$

Next, we use for $0 \leq n \leq 6$ the negative of these remainder integrals as input data in the recursive schemes (2.14), (3.9), and (4.14), and do a Taylor expansion of the resulting expressions. Thus, we obtain according to (2.13), (3.9), and (4.13)

$$\mathcal{A}_3^{(0)} = \frac{\ln(1+z)}{z} + \frac{421z^7}{16537500} - \frac{796321z^8}{8682187500} + \frac{810757427z^9}{4051687500000} + O(z^{10}), \tag{5.6a}$$

$$\varepsilon_6^{(0)} = \frac{\ln(1+z)}{z} + \frac{z^7}{9800} - \frac{31z^8}{77175} + \frac{113z^9}{120050} + O(z^{10}), \tag{5.6b}$$

$$\mathcal{J}_2^{(0)} = \frac{\ln(1+z)}{z} + \frac{z^7}{37800} - \frac{19z^8}{198450} + \frac{z^9}{4725} + O(z^{10}). \tag{5.6c}$$

All calculations were done symbolically, using the exact rational arithmetics of Maple. Consequently, the results in (5.6) are exact and free of rounding errors.

The leading coefficients of the Taylor expansions of the transformation error terms for $\mathcal{A}_3^{(0)}$ and $\mathcal{J}_2^{(0)}$ are evidently smaller than the corresponding coefficients for $\varepsilon_6^{(0)}$. This observation provides considerable evidence that Aitken’s iterated Δ^2 process and Brezinski’s iterated theta algorithm are in the case of the series (5.2) for $\ln(1+z)/z$ more effective than Wynn’s epsilon algorithm which according to (3.2) produces Padé approximants.

This conclusion is also confirmed by the following numerical example in Table 1, in which the convergence of the series (5.2) for $\ln(1+z)/z$ is accelerated for $z=0.95$. The numerical values of the

Table 1

Convergence of the transformation error terms. Transformation of $\ln(1+z)/z = \sum_{m=0}^{\infty} (-z)^m / (m+1)$ for $z = 0.95$

n	$\sum_{m=0}^{\infty} \frac{(-1)^{n+m} z^m}{n+m+2}$	$z^{n+1} R_{\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)}(z)$ Eq. (2.13)	$z^{n+1} r_{2\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)}(z)$ Eq. (3.9)	$z^{n+1} \mathcal{R}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)}(z)$ Eq. (4.13)
0	$0.312654 \cdot 10^0$	0	0	0
1	$-0.197206 \cdot 10^0$	0	0	0
2	$0.143292 \cdot 10^0$	$0.620539 \cdot 10^{-2}$	$0.620539 \cdot 10^{-2}$	0
3	$-0.112324 \cdot 10^0$	$-0.230919 \cdot 10^{-2}$	$-0.230919 \cdot 10^{-2}$	$0.113587 \cdot 10^{-2}$
4	$0.922904 \cdot 10^{-1}$	$0.109322 \cdot 10^{-3}$	$0.156975 \cdot 10^{-3}$	$-0.367230 \cdot 10^{-3}$
5	$-0.782908 \cdot 10^{-1}$	$-0.333267 \cdot 10^{-4}$	$-0.466090 \cdot 10^{-4}$	$0.148577 \cdot 10^{-3}$
6	$0.679646 \cdot 10^{-1}$	$0.131240 \cdot 10^{-5}$	$0.413753 \cdot 10^{-5}$	$0.137543 \cdot 10^{-5}$
7	$-0.600373 \cdot 10^{-1}$	$-0.371684 \cdot 10^{-6}$	$-0.108095 \cdot 10^{-5}$	$-0.392983 \cdot 10^{-6}$
8	$0.537619 \cdot 10^{-1}$	$0.111500 \cdot 10^{-7}$	$0.110743 \cdot 10^{-6}$	$0.131377 \cdot 10^{-6}$
9	$-0.486717 \cdot 10^{-1}$	$-0.311899 \cdot 10^{-8}$	$-0.266535 \cdot 10^{-7}$	$0.412451 \cdot 10^{-9}$
10	$0.444604 \cdot 10^{-1}$	$0.689220 \cdot 10^{-10}$	$0.298638 \cdot 10^{-8}$	$-0.139178 \cdot 10^{-9}$
11	$-0.409189 \cdot 10^{-1}$	$-0.199134 \cdot 10^{-10}$	$-0.678908 \cdot 10^{-9}$	$0.475476 \cdot 10^{-10}$
12	$0.378992 \cdot 10^{-1}$	$0.282138 \cdot 10^{-12}$	$0.808737 \cdot 10^{-10}$	$-0.316716 \cdot 10^{-12}$

remainder terms (5.5) were used as input data in the recursive schemes (2.14), (3.9), and (4.13) to compute numerically the transformation error terms in (2.13), (3.9), and (4.13). The transformation error terms, which are listed in columns 3–5, were chosen in agreement with (2.27), (3.21), and (4.26), respectively.

The zeros, which are found in columns 3–5 of Table 1, occur because Aitken’s iterated Δ^2 process and Wynn’s epsilon algorithm can only compute a rational approximant if at least three consecutive partial sums are available, and because the iteration of Brezinski’s theta algorithm requires at least four partial sums.

The result in Table 1 show once more that Aitken’s iterated Δ^2 process and Brezinski’s iterated theta algorithm are in the case of series (5.2) for $\ln(1+z)/z$ apparently more effective than Wynn’s epsilon algorithm.

The second group of results of this article — (2.19), (3.14), and (4.18) and the corresponding recursive schemes (2.20), (3.15), and (4.19) — can for example be used to demonstrate how rational approximants work if a divergent power series is to be summed.

Let us therefore assume that the partial sums, which occur in (2.19), (3.14), and (4.18), diverge if the index becomes large. Then, a summation to a finite generalized limit $f(z)$ can only be accomplished if $z^{n+2k+1} \Phi_k^{(n)}(z)$ and $z^{n+2k+1} \varphi_{2k}^{(n)}(z)$ in (2.19) and (3.14), respectively, converge to the negative of $f_{n+2k}(z)$, and if $z^{n+3k+1} \Psi_k^{(n)}(z)$ in (4.18) converges to the negative of $f_{n+3k}(z)$.

Table 2 shows that this is indeed the case. We again consider the infinite series (5.2) for $\ln(1+z)/z$, but this time we choose $z = 5.0$, which is clearly outside the circle of convergence. We use the numerical values of the partial sums $\sum_{m=0}^n (-z)^m / (m+1)$ with $0 \leq n \leq 10$ as input data in the recursive schemes (2.20), (3.15), and (4.19) to compute the transformation terms in (2.19), (3.14), and (4.18). The transformation terms, which are listed in columns 3–5 of Table 2, were chosen in agreement with (2.27), (3.21), and (4.26), respectively. All calculations were done using the floating point arithmetics of Maple.

Table 2

Convergence of transformation terms to the partial sums. Transformation of $\ln(1+z)/z = \sum_{m=0}^{\infty} (-z)^m/(m+1)$ for $z = 5.0$

n	$\sum_{m=0}^n \frac{(-z)^m}{m+1}$	$z^{n+1} \Phi_{\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)}(z)$ Eq. (2.19)	$z^{n+1} \varphi_{2\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)}(z)$ Eq. (3.14)	$z^{n+1} \Psi_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)}(z)$ Eq. (4.18)
0	$0.1000000000 \cdot 10^1$	0	0	0
1	$-0.1500000000 \cdot 10^1$	0	0	0
2	$0.6833333333 \cdot 10^1$	$-0.6410256410 \cdot 10^1$	$-0.6410256410 \cdot 10^1$	0
3	$-0.2441666667 \cdot 10^2$	$0.2467105263 \cdot 10^2$	$0.2467105263 \cdot 10^2$	$0.2480158730 \cdot 10^2$
4	$0.1005833333 \cdot 10^3$	$-0.1002174398 \cdot 10^3$	$-0.1002155172 \cdot 10^3$	$-0.1002604167 \cdot 10^3$
5	$-0.4202500000 \cdot 10^3$	$0.4205996885 \cdot 10^3$	$0.4205974843 \cdot 10^3$	$0.4206730769 \cdot 10^3$
6	$0.1811892857 \cdot 10^4$	$-0.1811533788 \cdot 10^4$	$-0.1811532973 \cdot 10^4$	$-0.1811533744 \cdot 10^4$
7	$-0.7953732143 \cdot 10^4$	$0.7954089807 \cdot 10^4$	$0.7954089068 \cdot 10^4$	$0.7954089765 \cdot 10^4$
8	$0.3544904563 \cdot 10^5$	$-0.3544868723 \cdot 10^5$	$-0.3544868703 \cdot 10^5$	$-0.3544868636 \cdot 10^5$
9	$-0.1598634544 \cdot 10^6$	$0.1598638127 \cdot 10^6$	$0.1598638125 \cdot 10^6$	$0.1598638127 \cdot 10^6$
10	$0.7279206365 \cdot 10^6$	$-0.7279202782 \cdot 10^6$	$-0.7279202781 \cdot 10^6$	$-0.7279202782 \cdot 10^6$

The results in Table 2 show that a sequence transformation accomplishes a summation of a divergent series by constructing approximations to the actual remainders. Both the partial sums as well as the actual remainders diverge individually if their indices become large, but the linear combination of the partial sum and the remainder has a constant and finite value for every index.

The fact, that the transformation terms in (2.19), (3.14), and (4.18) approach the negative of the corresponding partial sums of course also implies that one should not try to sum a divergent series in this way. The subtraction of two nearly equal terms would inevitably lead to a serious loss of significant digits.

In the next example, the transformation terms in (2.19), (3.14), and (4.18) will be used to make predictions for unknown series coefficients. For that purpose, it is recommendable to use a computer algebra system like Maple, and do all calculations symbolically. If the coefficients of the series to be transformed are exact rational numbers, the resulting rational expressions are then computed exactly.

We use the symbolic expressions for the partial sums $\sum_{m=0}^n (-z)^m/(m+1)$ with $0 \leq n \leq 12$ of the infinite series (5.2) for $\ln(1+z)/z$ as input data in the recursive schemes (2.20), (3.15), and (4.19). The resulting rational expressions $z^{13} \Phi_6^{(0)}(z)$, $z^{13} \varphi_{12}^{(0)}(z)$, and $z^{13} \Psi_4^{(4)}$ with unspecified z are then expanded, yielding predictions for the next series coefficients that are exact rational numbers. Only in the final step, the predictions for the next series coefficients are converted to floating point numbers in order to improve readability:

$$\begin{aligned} \mathcal{A}_6^{(0)} &= \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142857137 z^{13} + 0.06666666629 z^{14} \\ &\quad - 0.06249999856 z^{15} + 0.05882352524 z^{16} + O(z^{17}), \end{aligned} \tag{5.7a}$$

$$\begin{aligned} \mathcal{E}_{12}^{(0)} &= \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142854717 z^{13} + 0.06666649774 z^{14} \\ &\quad - 0.06249934843 z^{15} + 0.05882168762 z^{16} + O(z^{17}), \end{aligned} \tag{5.7b}$$

$$\mathcal{F}_4^{(0)} = \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142857148 z^{13} + 0.066666666684 z^{14} - 0.06249999986 z^{15} + 0.05882352708 z^{16} + O(z^{17}), \tag{5.7c}$$

$$\frac{\ln(1+z)}{z} = \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142857143 z^{13} + 0.066666666667 z^{14} - 0.06250000000 z^{15} + 0.05882352941 z^{16} + O(z^{17}). \tag{5.7d}$$

The accuracy of the prediction results in (5.7) is quite remarkable. The coefficients $\gamma_m = (-1)^m / (m+1)$ with $0 \leq m \leq 12$ are the only information that was used for the construction of the transformation terms $z^{13}\Phi_6^{(0)}(z)$, $z^{13}\varphi_{12}^{(0)}(z)$, and $z^{13}\Psi_4^{(0)}$, which were expanded to yield the results in (5.7). The accuracy of the approximations to the next four coefficients should suffice for many practical applications.

As in all other application, Wynn’s epsilon algorithm is in (5.7) slightly but significantly less effective than Aitken’s iterated Δ^2 process and Brezinski’s iterated theta algorithm.

Instead of computing the transformation terms $z^{13}\Phi_6^{(0)}(z)$, $z^{13}\varphi_{12}^{(0)}(z)$, and $z^{13}\Psi_4^{(0)}$, it is of course also possible to compute $\mathcal{A}_6^{(0)}$, $\varepsilon_{12}^{(0)}$, and $\mathcal{F}_4^{(0)}$ directly via their defining recursive schemes, and to expand the resulting rational expressions with a symbolic system like Maple. This would lead to the same results. However, in order to extract the partial sum $\sum_{m=0}^{12} (-z)^m / (m+1)$ from the rational approximants $\mathcal{A}_6^{(0)}$, $\varepsilon_{12}^{(0)}$, and $\mathcal{F}_4^{(0)}$, one would have to compute their 12th-order derivatives, and only the next derivatives would produce predictions to unknown series coefficients. Thus, this approach can easily become very expensive. In contrast, the use of the transformation terms requires only low-order derivatives of rational expressions.

If only the prediction of a single unknown term is to be done, then it is of course much more efficient to use the recursive schemes (2.23), (3.17), and (4.21). The input data of these recursive schemes are the coefficients of the series to be transformed, and no differentiations have to be done.

6. Summary and conclusions

As already mentioned in Section 1, it has become customary in certain branches of theoretical physics to use Padé approximants to make predictions for the leading unknown coefficients of strongly divergent perturbation expansions. This can be done by constructing symbolic expressions for Padé approximants from the known coefficients of the perturbation series. A Taylor expansion of sufficiently high order of such a Padé approximants then produces the predictions for the series coefficients which were not used for the construction of the Padé approximant. The Taylor expansion of the symbolic expression can be done comparatively easily with the help of powerful computer algebra systems like Maple or Mathematica, which are now commercially available for a wide range of computers.

It is the purpose of this article to overcome two principal shortcomings of the approach sketched above: Firstly, it is not necessary to rely entirely on the symbolic capabilities of computers. Instead, it is possible to construct recursive schemes, which either facilitate considerably the symbolic tasks computers have to perform, or which permit a straightforward computation of the prediction for

the leading unknown coefficient. Secondly, it is possible to use instead of Padé approximants other sequence transformations, as proposed by Sidi and Levin [85] and Brezinski [18]. It was shown in [105] that this may lead to more accurate predictions.

In this article, the prediction properties of Aitken's iterated Δ^2 process, Wynn's epsilon algorithm, and Brezinski's iterated theta algorithm are studied.

As is well known [4,8], a Padé approximant can be considered to be the solution of a system of linear equations for the coefficients of its numerator and denominator polynomials. If this system of linear equations has a solution, then it is automatically guaranteed that the Padé approximant satisfies the accuracy-through-order relationship (1.6). In the case of other sequence transformations, the situation is usually much more difficult. They are usually not defined as solutions of systems of linear equations, but via (complicated) nonlinear recursive schemes.

Since accuracy-through-order relationships of the type of (1.6) play a very important role for the understanding of the prediction properties of sequence transformations, it was necessary to derive accuracy-through-order relationships for Aitken's iterated Δ^2 process, Wynn's epsilon algorithm, and Brezinski's iterated theta algorithm on the basis of their defining recursive schemes.

Unfortunately, the defining recursive schemes (2.4), (3.1), and (4.3) are not suited for a construction of accuracy-through-order relationships. They first had to be modified appropriately, yielding the mathematically equivalent recursive schemes (2.11), (3.8), and (4.11).

These alternative recursive schemes were the starting point for the derivation of the accuracy-through-order relationships (2.13), (3.9), and (4.13) and the corresponding recursive schemes (2.14), (3.10), and (4.14) for the transformation error terms. These relationships describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\varepsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the function $f(z)$ which is to be approximated.

With the help of these accuracy-through-order relationships, a second group of results could be derived — (2.19), (3.14), and (4.18) and the corresponding recursive schemes (2.20), (3.15), and (4.19) — which describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\varepsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the partial sums which were used for their construction. These differences are expressed by the terms $z^{n+2k+1}\Phi_k^{(n)}(z)$, $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$, and $z^{n+3k+1}\Psi_k^{(n)}(z)$ which can be computed via the recursive schemes (2.20), (3.15), and (4.19).

The predictions for the leading unknown series coefficients can be obtained by expanding symbolic expressions for these transformation terms. The advantage of this approach is that the partial sums, which are used for the construction of the rational approximants $\mathcal{A}_k^{(n)}$, $\varepsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ as well as of the transformation terms $z^{n+2k+1}\Phi_k^{(n)}(z)$, $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$, and $z^{n+3k+1}\Psi_k^{(n)}(z)$, are already explicitly separated. Consequently, only derivatives of low order have to be computed. Moreover, the predictions for the leading unknown series coefficient can be computed conveniently via the recursive schemes (2.23), (3.17), and (4.21). In this way, it is neither necessary to construct symbolic expressions nor to differentiate them.

Finally, in Section 5 some applications of the new results were presented. In all applications of this article, Wynn's epsilon algorithm was found to be less effective than Aitken's iterated Δ^2 process or Brezinski's iterated theta algorithm. Of course, it remains to be seen whether this observation is specific for the infinite series (5.2) for $\ln(1+z)/z$, which was used as the test system, or whether it is actually more generally valid. Nevertheless, the results presented in Section 5 provide further evidence that suitably chosen sequence transformations may indeed be more effective than Padé approximants. Consequently, one should not assume that Padé approximants produce by default the best results in convergence acceleration and summation processes, and it may well be worth while to

investigate whether sequence transformations can be found which are better adapted to the problem under consideration.

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