Construction of New Generalizations of Wynn's Epsilon and Rho Algorithm by Solving Finite Difference Equations in the Transformation Order

Xiang-Ke Chang · Yi He · Xing-Biao Hu · Jian-Qing Sun · Ernst Joachim Weniger

To Appear in Numerical Algorithms: March 26, 2019

Abstract We construct new sequence transformations based on Wynn's epsilon and rho algorithms. The recursions of the new algorithms include the recursions of Wynn's epsilon and rho algorithm and of Osada's generalized rho algorithm as special cases. We demonstrate the performance of our algorithms numerically by applying them to some linearly and logarithmically convergent sequences as well as some divergent series.

Keywords convergence acceleration algorithm, sequence transformation, epsilon algorithm, rho algorithm

Mathematics Subject Classification (2010) Primary 65B05, 65B10

We dedicate this article to the memory of Peter Wynn (1931 - 2017)

Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, PR China E-mail: heyi@wipm.ac.cn

Xing-Biao Hu

LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, P.O.Box 2719, Beijing 100190, PR China; and School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, PR China E-mail: hxb@lsec.cc.ac.cn

Jian-Qing Sun

School of Mathematical Sciences, Ocean University of China, Qingdao, 266100, PR China E-mail: sunjq@lsec.cc.ac.cn

Ernst Joachim Weniger

Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Germany E-mail: joachim.weniger@chemie.uni-regensburg.de

Xiang-Ke Chang

LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, P.O.Box 2719, Beijing 100190, PR China; and School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, PR China E-mail: changxk@lsec.cc.ac.cn

Yi He

Contents

1	Introduction	3
2	Review of Wynn's epsilon and rho algorithm and of related transformations	6
	2.1 The Shanks transformation and Wynn's epsilon algorithm	6
	2.2 Wynn's rho algorithm	8
	2.3 Brezinski's theta algorithm and its iteration	10
3	Difference equations with respect to the transformation order	12
	3.1 General Considerations	12
	3.2 First order difference equations	13
	3.3 Second order difference equations	14
	3.4 Initial conditions for the new transformation	15
4	Numerical examples	17
	4.1 Asymptotic model sequences	17
	4.2 Linearly convergent sequences	18
	4.3 Logarithmically convergent sequences	19
	4.4 Divergent series	21
5	Conclusions and discussions	23
Аŗ	opendices	25
А	Reduced Bessel functions	25
В	Levin's transformation	26
	B.1 The general Levin transformation	26
	B.2 Levin's <i>u</i> transformation	27
	B.3 Levin's v transformation	28
Bi	bliography	32

1 Introduction

Sequences and series are extremely important mathematical tools. They appear naturally in many methods for solving differential and integral equations, in discretization methods, in quadrature schemes, in perturbation techniques, or in the evaluation of special functions. Unfortunately, the resulting sequences or series often do not converge fast enough to be practically useful, or they even diverge, which means that summation techniques have to be employed to obtain numerically useful information. In such situations, it is often helpful to employ so-called sequence transformations.

Formally, a sequence transformation \mathcal{T} is simply a map

$$\mathscr{T}: \{S_n\} \to \{T_n\}, \qquad n \in \mathbb{N}_0, \tag{1.1}$$

which transforms a given sequence $\{S_n\}$, whose convergence may be unsatisfactory, to a new sequence $\{T_n\}$ with hopefully better numerical properties. Of course, there is the minimal requirement that the transformed sequence $\{T_n\}$ must have the same (generalized) limit *S* as the original sequence $\{S_n\}$, but otherwise we have a lot of freedom. It is common to say that \mathscr{T} accelerates convergence if $\{T_n\}$ converges more rapidly to *S* than $\{S_n\}$ according to

$$\lim_{n \to \infty} \frac{T_n - S}{S_n - S} = 0. \tag{1.2}$$

Many practically relevant sequences can be classified according to some simple convergence types. Let us assume that the elements of a sequence $\{S_n\}$ with (generalized) limit *S* satisfy the following criterion resembling the well known ratio test:

$$\lim_{n \to \infty} \frac{S_{n+1} - S}{S_n - S} = \rho.$$
(1.3)

If $0 < |\rho| < 1$ holds, $\{S_n\}$ converges *linearly*, if $\rho = 1$ holds, $\{S_n\}$ converges *logarithmically*, and if $\rho = 0$ holds, it converges *hyperlinearly*. Obviously, $|\rho| > 1$ implies divergence. The partial sums $\sum_{k=0}^{n} z^k = [1 - z^{n+1}]/[1 - z]$ of the geometric series converge linearly for |z| < 1 as $n \to \infty$, and they diverge for $|z| \ge 1$. The partial sums $\sum_{k=0}^{n} (k+1)^{-s}$ of the Dirichlet series $\zeta(s) = \sum_{\nu=0}^{\infty} (\nu+1)^{-s}$ for the Riemann zeta function converge logarithmically for $\Re(s) > 1$ (see for example [98, Eq. (2.6)]), and the partial sums $\sum_{k=0}^{n} z^k / k!$ of the power series for $\exp(z)$ converge hyperlinearly for $z \in \mathbb{C}$.

A sequence transformation \mathscr{T} corresponds to an infinite set of doubly indexed quantities $T_k^{(n)}$ with $k, n \in \mathbb{N}_0$. Each $T_k^{(n)}$ is computed from a *finite* subset $\{S_n, S_{n+1}, \ldots, S_{n+\ell(k)}\}$ of *consecutive* elements, where $\ell = \ell(k)$. In our notation, $T_0^{(n)}$ always corresponds to an untransformed sequence element $T_0^{(n)} = S_n$.

The *transformation order k* is a measure for the complexity of $T_k^{(n)}$, and the superscript *n* corresponds to the minimal index *n* of the string $\{S_n, S_{n+1}, \ldots, S_{n+\ell(k)}\}$ of input data. An increasing value of *k* implies that the complexity of the transformation process as well as $\ell = \ell(k)$ increases. Thus, the application of a sequence transformation \mathscr{T} to $\{S_n\}$ produces for every $k, n \geq \mathbb{N}_0$ a new transformed element

$$T_k^{(n)} = T_k^{(n)} \left(S_n, S_{n+1}, \dots, S_{n+\ell(k)} \right).$$
(1.4)

Sequence transformations are at least as old as calculus, and in rudimentary form they are even much older. For the older history of sequence transformations, we recommend a monograph by Brezinski [23], which discusses earlier work on continued fractions, Padé

approximants, and related topics starting from the 17th century until 1945, as well as an article by Brezinski [26], which emphasizes pioneers of extrapolation methods. More recent developments are treated in articles by Brezinski [24, 25, 27] and Brezinski and Redivo Za-glia [29]. A very complete list of older references up to 1991 can be found in a bibliography by Brezinski [22].

Ever since the pioneering work of Shanks [69] and Wynn [101], respectively, *nonlin-ear* and in general also *nonregular* sequence transformations have dominated both research and practical applications. For more details, see the monographs by Brezinski [19, 20, 21], Brezinski and Redivo Zaglia [28], Cuyt and Wuytack [37], Delahaye [38], Liem, Lü, and Shih [56], Marchuk and Shaidurov [57], Sidi [73], Walz [85], and Wimp [100], or articles by Caliceti, Meyer-Hermann, Ribeca, Surzhykov, and Jentschura [34], Homeier [52], and Weniger [88]. Sequence transformations are also treated in the book by Baker and Graves-Morris [2] on Padé approximants, which can be viewed to be just a special class of sequence transformations since they convert the partial sums of a power series to a doubly indexed sequence of rational functions.

Practical applications of sequence transformations are emphasized in a book by Bornemann, Laurie, Wagon, and Waldvogel [14, Appendix A] on extreme digit hunting, in the most recent (third) edition of the book *Numerical Recipes* [65] (a review of the treatment of sequence transformations in *Numerical Recipes* by Weniger [94] can be downloaded from the Numerical Recipes web page), in a book by Gil, Segura, and Temme [45] on the evaluation of special functions (compare also the related review articles by Gil, Segura, and Temme [46] and by Temme [79]), in the recently published NIST Handbook of Mathematical Functions [59, Chapter 3.9 Acceleration of Convergence], and in a recent book by Trefethen [82] on approximation theory. Readers interested in current research both on and with sequence transformations might look into the proceedings of a recent conference [30, 97].

Certain sequence transformations are closely related to dynamical systems. For example, Wynn's epsilon [101] and rho [102] algorithm can be viewed to be just fully discrete integrable systems [58, 64]. New sequence transformations were also derived via this connection with dynamical systems [31, 35, 51, 77].

It is the basic assumption of all the commonly used sequence transformations that the elements S_n of a given sequence $\{S_n\}$ can be partitioned into a (generalized) limit S and a remainder R_n according to

$$S_n = S + R_n, \qquad n \in \mathbb{N}_0. \tag{1.5}$$

How do sequence transformations accomplish an acceleration of convergence or a summation of a divergent sequence? Let us assume that some sufficiently good approximations $\{\tilde{R}_n\}$ to the actual remainders $\{R_n\}$ of the elements of the sequence $\{S_n\}$ are known. Elimination of these approximations \tilde{R}_n yields a new sequence

$$S'_{n} = S_{n} - \tilde{R}_{n} = S + R_{n} - \tilde{R}_{n} = S + R'_{n}.$$
(1.6)

If \tilde{R}_n is a good approximation to R_n , the transformed remainder $R'_n = R_n - \tilde{R}_n$ vanishes more rapidly than the original remainders R_n as $n \to \infty$. At least conceptually, this is what a sequence transformation tries to accomplish, although it may actually use a completely different computational algorithm. Thus, when trying to construct a new sequence transformation, we have to look for arithmetic operations that lead in each step to an improved approximate elimination of the truncation errors.

The idea of viewing a sequence transformation as an approximate elimination procedure for the truncation errors becomes particularly transparent in the case of model sequences whose remainders R_n consists of a single exponential term:

$$S_n = S + C\lambda^n, \qquad C \neq 0, \quad |\lambda| < 1, \quad n \in \mathbb{N}_0.$$
(1.7)

This is an almost trivially simple model problem. Nevertheless, many practically relevant sequences are known where exponential terms of the type of $C\lambda^n$ form the dominant parts of their truncation errors.

A short computation shows that the so-called Δ^2 formula (see for example [88, Eq. (5.1-4)])

$$\mathscr{A}_{1}^{(n)} = S_{n} - \frac{[\Delta S_{n}]^{2}}{\Delta^{2} S_{n}}, \qquad n \in \mathbb{N}_{0}, \qquad (1.8)$$

is exact for the model sequence (1.7), i.e., we have $\mathscr{A}_1^{(n)} = S$. Here, Δ is the finite difference operator defined by $\Delta f(n) = f(n+1) - f(n)$.

Together with its numerous mathematically, but not necessarily numerically equivalent explicit expressions (see for example [88, Eqs. (5.1-6) - (5.1-12)]), the Δ^2 formula (1.8) is commonly attributed to Aitken [1], although it is in fact much older. Brezinski [23, 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 the Δ^2 formula (see also Osada's article [62, Section 5]), and according to Todd [80, p. 5], the Δ^2 formula was in principle known to Kummer [53] already in 1837.

The power and practical usefulness of the Δ^2 formula (1.8) is obviously limited since it only eliminates a single exponential term. However, the Δ^2 formula (1.8) can be iterated by using the output data $\mathscr{A}_1^{(n)}$ as input data in the Δ^2 formula. Repeating this process yields the following nonlinear recursive scheme (see for example [88, Eq. (5.1-15)]):

$$\mathscr{A}_0^{(n)} = S_n, \qquad n \in \mathbb{N}_0, \tag{1.9a}$$

$$\mathscr{A}_{k+1}^{(n)} = \mathscr{A}_{k}^{(n)} - \frac{\left[\Delta \mathscr{A}_{k}^{(n)}\right]^{2}}{\Delta^{2} \mathscr{A}_{k}^{(n)}}, \qquad k, n \in \mathbb{N}_{0}.$$

$$(1.9b)$$

Here, Δ only acts on the superscript *n* but not on the subscript *k* according to $\Delta \mathscr{A}_k^{(n)} = \mathscr{A}_k^{(n+1)} - \mathscr{A}_k^{(n)}$ (if necessary, we write $\Delta_n \mathscr{A}_k^{(n)}$ for the sake of clarity). The iterated Δ^2 process (1.9) is a fairly powerful sequence transformation (see for exam-

The iterated Δ^2 process (1.9) is a fairly powerful sequence transformation (see for example [88, Table 13-1 on p. 328 or Section 15.2]). In [88, p. 228], one finds the listing of a FOR-TRAN 77 program that computes the iterated Δ^2 process using a single one-dimensional array.

There is an extensive literature on both the Δ^2 formula (1.8) and its iteration (1.9) (see for example [29, 92] and references therein). But it is even more important that Aitken paved the way for the Shanks transformation [70] and for Wynn's epsilon algorithm [101], which permits a convenient recursive computation of the Shanks transformation and thus also of Padé approximants. In 1956, Wynn also derived his so-called rho algorithm [102], whose recursive scheme closely resembles that of the epsilon algorithm. These well known facts will be reviewed in more detail in Section 2.

The aim of our article is the clarification of the relationships among known generalizations of Wynn's epsilon [101] and rho [102] algorithms, and the construction of new generalizations. We accomplish this by considering finite difference equations in the transformation order k. To the best of our knowledge, this is a novel approach. It leads to a better understanding of the epsilon and rho algorithm and of many of their generalizations. In addition, our approach also produces several new sequence transformations. It would be overly optimistic to assume that this article, which is the first one to describe and apply our novel approach, could provide definite answers to all questions occurring in this context. We also do not think that the new transformations, which are presented in this article, exhaust the potential of our novel approach.

The details of our novel approach will be discussed in Section 3. In Section 4, we will show the performance of our algorithms by some numerical examples. Finally, Section 5 is devoted to discussions and conclusions.

2 Review of Wynn's epsilon and rho algorithm and of related transformations

2.1 The Shanks transformation and Wynn's epsilon algorithm

An obvious generalization of the model sequence (1.7), which leads to the Δ^2 formula (1.8), is the following one, which contains *k* exponential terms instead of one:

$$S_n = S + \sum_{j=0}^{k-1} C_j(\lambda_j)^n, \qquad k, n \in \mathbb{N}_0.$$
 (2.1)

It is usually assumed that the λ_j are distinct $(\lambda_m \neq \lambda_n \text{ for } m \neq n)$, and that they ordered according to magnitude $(|\lambda_0| > |\lambda_1| > \cdots > |\lambda_{k-1}|)$.

Although the Δ^2 formula (1.8) is by construction exact for the model sequence (1.7), its iteration (1.9) with k > 1 is not exact for the model sequence (2.1). Instead, the Shanks transformation, which is defined by the following ratio of Hankel determinants [70, Eq. (2)],

$$e_{k}(S_{n}) = \frac{\begin{vmatrix} S_{n} & S_{n+1} & \dots & S_{n+k} \\ \Delta S_{n} & \Delta S_{n+1} & \dots & \Delta S_{n+k} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta S_{n+k-1} & \Delta S_{n+k} & \dots & \Delta S_{n+2k-1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \dots & 1 \\ \Delta S_{n} & \Delta S_{n+1} & \dots & \Delta S_{n+k} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta S_{n+k-1} & \Delta S_{n+k} & \dots & \Delta S_{n+2k-1} \end{vmatrix}}, \qquad k, n \in \mathbb{N}_{0}.$$
(2.2)

is exact for the model sequence (2.1). Actually, the Shanks transformation had originally been derived in 1941 by Schmidt [67], but Schmidt's article had largely been ignored.

Shanks' discovery of his transformation (2.2) had an enormous impact, in particular since he could show that it produces Padé approximants. Let

$$f_n(z) = \sum_{\nu=0}^n \gamma_{\nu} z^{\nu}, \qquad n \in \mathbb{N}_0, \qquad (2.3)$$

stand for the partial sums of the (formal) power series for some function f. Then [70, Theorem VI on p. 22],

$$e_k(f_n(z)) = [k+n/k]_f(z), \qquad k, n \in \mathbb{N}_0.$$
(2.4)

We use the notation of Baker and Graves-Morris [2, Eq. (1.2)] for Padé approximants.

The Hankel determinants in Shanks' transformation (2.2) can be computed recursively via the following non-linear recursion (see for example [28, p. 80]:

$$H_0(u_n) = 1, \qquad H_1(u_n) = u_n, \qquad n \in \mathbb{N}_0,$$
 (2.5a)

$$H_{k+2}(u_n)H_k(u_{n+2}) = H_{k+1}(u_n)H_{k+1}(u_{n+2}) - [H_{k+1}(u_{n+1})]^2, \qquad k, n \in \mathbb{N}_0.$$
 (2.5b)

This recursive scheme is comparatively complicated. Therefore, Wynn's discovery of his celebrated epsilon algorithm was a substantial step forwards [101, Theorem on p. 91]:

$$\varepsilon_{-1}^{(n)} = 0, \qquad \varepsilon_{0}^{(n)} = S_{n}, \qquad n \in \mathbb{N}_{0},$$
(2.6a)

$$\varepsilon_{k+1}^{(n)} = \varepsilon_{k-1}^{(n+1)} + \frac{1}{\varepsilon_{k}^{(n+1)} - \varepsilon_{k}^{(n)}}, \quad k, n \in \mathbb{N}_{0},$$
(2.6b)

Wynn [101, Theorem on p. 91] showed that the epsilon elements with *even* subscripts give Shanks' transformation

$$\varepsilon_{2k}^{(n)} = e_k(S_n), \qquad k, n \in \mathbb{N}_0, \tag{2.7}$$

whereas the elements with odd subscripts are only auxiliary quantities

$$\varepsilon_{2k+1}^{(n)} = 1/e_k(\Delta S_n), \qquad k, n \in \mathbb{N}_0,$$
(2.8)

which diverge if the transforms (2.7) converge to the (generalized) limit *S* of $\{S_n\}$.

The epsilon algorithm is a close relative of Aitken's iterated Δ^2 process. We have $\mathscr{A}_1^{(n)} = \varepsilon_2^{(n)}$, but for k > 1 we in general have $\mathscr{A}_k^{(n)} \neq \varepsilon_{2k}^{(n)}$. Nevertheless, the iterated Δ^2 process and the epsilon algorithm often have similar properties in convergence acceleration and summation processes.

Because of the rhombus structure of the four-term recursion (2.6b), it appears that a program for Wynn's epsilon algorithm would need either a single two-dimensional or at least two one-dimensional arrays. However, Wynn [103] could show with the help of his *moving lozenge technique*, which is described in a very detailed way in [20, Chapter 4.2.1.2], that a single one-dimensional array plus two auxiliary variables suffice. In [20, Chapter 4.3.2], one finds listings of several FORTRAN 66 programs for the epsilon algorithm.

As shown in [88, Section 4.3], a slight improvement of Wynn's moving lozenge technique is possible. The listing of a compact FORTRAN 77 program for the epsilon algorithm using this modification can be found in [88, p. 222]. In the book by Press, Teukolsky, Vetterling, and Flannery [65, p. 213], one finds a translation of this FORTRAN 77 program to C.

It follows from Eqs. (2.4) and (2.7) that the epsilon algorithm produces Padé approximants if its input data S_n are the partial sums (2.3) of a power series:

$$\boldsymbol{\varepsilon}_{2k}^{(n)} = [k + n/k]_f(z), \qquad k, n \in \mathbb{N}_0.$$
(2.9)

Consequently, the epsilon algorithm is treated in books on Padé approximants such as the one by Baker and Graves-Morris [2], but there is also an extensive literature dealing directly with it. According to Wimp [100, p. 120], 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 [19]. However, this book was published in 1977, and since then many more books and articles dealing with the epsilon algorithm have been published. Any attempt of providing a reasonably complete bibliography would be beyond the scope of this article.

The epsilon algorithm is not limited to input data that are the partial sums of a (formal) power series. Therefore, it is actually more general than Padé approximants. For example, sequences of vectors can be used as input data. For a relatively recent review, see [47]. Both Shanks' transformation and the epsilon algorithm are discussed in the NIST Handbook of Mathematical Functions [59, Chapter 3.9(iv) Shanks' Transformation].

Several generalizations of the epsilon algorithm are known. In 1972, Brezinski [18, pp. 72 and 78] introduced what he called his first and second generalization of the epsilon algorithm (see also [28, Chapter 2.6]). Sablonniere [66, Algorithm A1 on p. 180] and Sedogbo [68, Algorithm 1 and Theorem 1 on p. 255] introduced other generalizations of the epsilon algorithms that were specially designed to be effective for certain logarithmically convergent interation sequences. Other generalizations were considered by Vanden Broeck and Schwartz [84, Eq. (2.1)] and by Barber and Hamer [5, Eqs. (43) - (44)].

2.2 Wynn's rho algorithm

The iterated Δ^2 process (1.9) and the epsilon algorithm (2.6) are powerful accelerators for linearly convergent sequences, and they are also able to sum many alternating divergent series (see for example [88, Section 15.2] or the rigorous convergence analysis of the summation of the Euler series in [13]). However, both fail in the case of logarithmic convergence [104, Theorem 12]. Fortunately, in 1956 Wynn also derived his rho algorithm [102, Eq. (8)]

$$\rho_{-1}^{(n)} = 0, \qquad \rho_0^{(n)} = S_n, \qquad n \in \mathbb{N}_0,$$
(2.10a)

$$\rho_{k+1}^{(n)} = \rho_{k-1}^{(n+1)} + \frac{x_{n+k+1} - x_n}{\rho_k^{(n+1)} - \rho_k^{(n)}}, \qquad k, n \in \mathbb{N}_0,$$
(2.10b)

which is – as for example emphasized by Osada [61] – an effective accelerator for many logarithmically convergent sequences.

As in the case of the formally almost identical epsilon algorithm, only the elements $\rho_{2k}^{(n)}$ with *even* subscripts provide approximations to the limit of the input sequence. The elements $\rho_{2k+1}^{(n)}$ with *odd* subscripts are only auxiliary quantities which diverge if the transformation process converges. Actually, the elements $\rho_{2k}^{(n)}$ correspond to the terminants of an interpolating continued fraction with interpolation points $\{x_n\}$ that are extrapolated to infinity (see for example [37, Chapter IV.1.4]). Consequently, the interpolation points $\{x_n\}$ must be positive, strictly increasing, and unbounded:

$$0 < x_0 < x_1 < \dots < x_m < x_{m+1} < \dots,$$
 (2.11a)

$$\lim_{n \to \infty} x_n = \infty. \tag{2.11b}$$

In the vast majority of all applications, Wynn's rho algorithm (2.10) is used in combination with the interpolation points $x_n = n + 1$, yielding its standard form (see for example [88, Eq. (6.2-4)]):

$$\rho_{-1}^{(n)} = 0, \qquad \rho_0^{(n)} = S_n, \qquad n \in \mathbb{N}_0,$$
(2.12a)

$$\rho_{k+1}^{(n)} = \rho_{k-1}^{(n+1)} + \frac{k+1}{\rho_k^{(n+1)} - \rho_k^{(n)}}, \qquad k, n \in \mathbb{N}_0.$$
(2.12b)

The standard form (2.12) is not able to accelerate the convergence of *all* logarithmically convergent sequences of interest. This can be demonstrated by considering the following class of logarithmically convergent model sequences:

$$S_n = S + (n+\beta)^{-\theta} \sum_{j=0}^{\infty} c_j / (n+\beta)^j, \qquad n \in \mathbb{N}_0.$$
 (2.13)

Here, θ is a positive decay parameter and β is a positive shift parameter. The elements of numerous practically relevant logarithmically convergent sequences $\{S_n\}$ can at least in the asymptotic domain of large indices *n* be represented by series expansions of that kind.

Osada [60, Theorem 3.2] showed that the standard form (2.12) accelerates the convergence of sequences of the type of Eq. (2.13) if the decay parameter θ is a positive integer, but it fails if θ is non-integral.

If the decay parameter θ of a sequence of the type of Eq. (2.13) is explicitly known, Osada's variant of the rho algorithm can be used [60, Eq. (3.1)]:

$$\bar{\rho}_{-1}^{(n)} = 0, \qquad \bar{\rho}_{0}^{(n)} = S_n, \qquad n \in \mathbb{N}_0,$$
(2.14a)

$$\bar{\rho}_{k+1}^{(n)} = \bar{\rho}_{k-1}^{(n+1)} + \frac{k+\theta}{\bar{\rho}_{k}^{(n+1)} - \bar{\rho}_{k}^{(n)}}, \qquad k, n \in \mathbb{N}_{0}.$$
(2.14b)

Osada showed that his variant (2.14) accelerates the convergence of sequences of the type of Eq. (2.13) for known, but otherwise arbitrary, i.e., also for non-integral $\theta > 0$. He proved the following asymptotic estimate for fixed *k* [60, Theorem 4]:

$$\bar{\rho}_{2k}^{(n)} - S = \mathcal{O}\left(n^{-\theta - 2k}\right), \qquad n \to \infty.$$
(2.15)

As remarked above, the decay parameter θ must be explicitly known if Osada's transformation (2.14) is to be applied to a sequence of the type of Eq. (2.13). An approximation to θ can be obtained with the help of the following nonlinear transformation, which was first derived in a somewhat disguised form by Drummond [39, p. 419] and later rederived by Bjørstad, Dahlquist, and Grosse [11, Eq. (4.1)]:

$$T_{n} = \frac{[\Delta^{2}S_{n}][\Delta^{2}S_{n+1}]}{[\Delta S_{n+1}][\Delta^{2}S_{n+1}] - [\Delta S_{n+2}][\Delta^{2}S_{n}]} - 1, \qquad n \in \mathbb{N}_{0}.$$
(2.16)

Bjørstad, Dahlquist, and Grosse [11, Eq. (4.1)] showed that

$$\theta = T_n + O(1/n^2), \qquad n \to \infty, \tag{2.17}$$

if the input data are the elements of a sequence of the type of Eq. (2.13).

The variants of Wynn's rho algorithm can also be iterated in the spirit of Aitken's iterated Δ^2 process (1.9), which can also be viewed to be an iteration of $\varepsilon_2^{(n)}$. By iterating the expression for $\rho_2^{(n)}$ involving unspecified interpolation points x_n , a rho analog of Aitken's iterated Δ^2 was constructed [89, Eq. (2.10)]. An alternative iteration was derived by Bhowmick, Bhattacharya, and Roy [9, Eq. (2.25)], which is, however, significantly less efficient than the iteration [89, Eq. (2,10)] involving unspecified interpolation points (compare [89, Table I]). This is caused by the fact that Bhowmick, Bhattacharya, and Roy [9, Eq. (2.25)] had started from the standard form (2.12) and not from the general form (2.10). Osada's variant (2.14) of the rho algorithm can also be iterated. It yields a recursive scheme [89, Eq. (2.29)], which was originally derived by Bjørstad, Dahlquist, and Grosse [11, Eq. (2.4)] who called the resulting algorithm a modified Δ^2 formula.

Wynn's epsilon algorithm (2.6) is undoubtedly the currently most important and most often employed sequence transformation. Wynn's rho algorithm (2.10) and its standard form (2.12), Osada's generalized rho algorithm (2.14), as well as the iterations mentioned above are also very important and practically useful sequence transformations. Accordingly, there are numerous references describing successful applications (far too many to be cited here). In addition, these transformations were very consequential from a purely theoretical point of view. They inspired the derivation of numerous other sequence transformations and ultimately also this article.

2.3 Brezinski's theta algorithm and its iteration

Soon after their derivation it had become clear that epsilon and rho have largely complementary properties. The epsilon algorithm is a powerful accelerator of linear convergence and also frequently works well in the case of divergent series, but it does not accomplish anything substantial in the case of logarithmic convergence. In contrast, the rho algorithm is ineffective in the case of linear convergence and even more so in the case of divergent series, but is able to speed up the convergence of many logarithmically convergent sequences.

This observation raised the question whether it would be possible to modify the recursions of epsilon and/or rho in such a way that the resulting transformation would possess the advantageous features of both epsilon and rho. This goal was achieved in 1971 by Brezinski who suitably modified the epsilon recursion (2.6) to obtain his theta algorithm [16, p. 729] (compare also [28, Chapter 2.3] or [88, Section 10.1]):

$$\vartheta_{-1}^{(n)} = 0, \qquad \vartheta_0^{(n)} = S_n, \qquad n \in \mathbb{N}_0, \qquad (2.18a)$$

$$\vartheta_{2k+1}^{(n)} = \vartheta_{2k-1}^{(n+1)} + \frac{1}{\Delta \vartheta_{2k}^{(n)}}, \qquad k, n \in \mathbb{N}_0,$$
(2.18b)

$$\vartheta_{2k+2}^{(n)} = \vartheta_{2k}^{(n+1)} + \frac{\left[\Delta \vartheta_{2k}^{(n+1)}\right] \left[\Delta \vartheta_{2k+1}^{(n+1)}\right]}{\Delta^2 \vartheta_{2k+1}^{(n)}}, \qquad k, n \in \mathbb{N}_0.$$
(2.18c)

We again assume that the finite difference operator Δ only acts on *n* but not on *k*.

As in the case of Wynn's epsilon and rho algorithm, only the elements $\vartheta_{2k}^{(n)}$ with even subscripts provide approximations to the (generalized) limit of the sequence $\{S_n\}$ to be transformed. The elements $\vartheta_{2k+1}^{(n)}$ with odd subscripts are only auxiliary quantities which diverge if the whole process converges.

Brezinski's derivation of his theta algorithm was purely experimental, but it was certainly a very successful experiment. Extensive numerical studies performed by Smith and Ford [74, 75] showed that among virtually all sequence transformations known at that time only the theta algorithm together with Levin's u and v transformations [55, Eqs. (59) and (68)] provided consistently good results for a very wide range of test problems. This positive verdict was also confirmed by later numerical studies.

In Brezinski's second book [20, pp. 368 - 370], one finds the listing of a FORTRAN IV program which computes Brezinski's theta algorithm 2.18 using three one-dimensional arrays, and in [88, pp. 279 - 281], one finds the listing of a FORTRAN 77 program which computes theta using two one-dimensional arrays.

It is possible to proceed in the spirit of Aitken's iterated Δ^2 process (1.9) and to construct iterations of Brezinski's theta algorithm (2.18). A natural starting point for such an iteration

would be $\vartheta_2^{(n)}$ which possesses many alternative expressions (see for example [88, Eqs. (10.3-1) - (10.3-3)] or [92, Eq. (4.10)]):

$$\vartheta_{2}^{(n)} = S_{n+1} - \frac{\left[\Delta S_{n}\right] \left[\Delta S_{n+1}\right] \left[\Delta^{2} S_{n+1}\right]}{\left[\Delta S_{n+2}\right] \left[\Delta^{2} S_{n}\right] - \left[\Delta S_{n}\right] \left[\Delta^{2} S_{n+1}\right]}$$
(2.19)

$$=\frac{S_{n+1}[\Delta S_{n+2}][\Delta^2 S_n] - S_{n+2}[\Delta S_n][\Delta^2 S_{n+1}]}{[\Delta S_{n+2}][\Delta^2 S_n] - [\Delta S_n][\Delta^2 S_{n+1}]}$$
(2.20)

$$=\frac{\Delta^2 [S_{n+1}/\Delta S_n]}{\Delta^2 [1/\Delta S_n]}$$
(2.21)

$$= S_{n+3} - \frac{\left[\Delta S_{n+2}\right] \left\{ \left[\Delta S_{n+2}\right] \left[\Delta^2 S_n\right] + \left[\Delta S_{n+1}\right]^2 - \left[\Delta S_{n+2}\right] \left[\Delta S_n\right] \right\}}{\left[\Delta S_{n+2}\right] \left[\Delta^2 S_n\right] - \left[\Delta S_n\right] \left[\Delta^2 S_{n+1}\right]}.$$
 (2.22)

As in the case of $\mathscr{A}_2^{(n)}$, these expressions are obviously mathematically equivalent, but they may differ – possibly substantially – with respect to their numerical stability.

By iterating the explicit expression (2.19) for $\vartheta_2^{(n)}$ in the spirit of Aitken's iterated Δ^2 process (1.9), the following nonlinear recursive system was derived [88, Eq. (10.3-6)]:

$$\begin{aligned}
\mathcal{J}_{0}^{(n)} &= S_{n}, \qquad n \in \mathbb{N}_{0}, \\
\mathcal{J}_{k+1}^{(n)} &= \mathcal{J}_{k}^{(n+1)} - \frac{\left[\Delta \mathcal{J}_{k}^{(n)}\right] \left[\Delta \mathcal{J}_{k}^{(n+1)}\right] \left[\Delta^{2} \mathcal{J}_{k}^{(n+1)}\right]}{\left[\Delta \mathcal{J}_{k}^{(n+2)}\right] \left[\Delta^{2} \mathcal{J}_{k}^{(n)}\right] - \left[\Delta \mathcal{J}_{k}^{(n)}\right] \left[\Delta^{2} \mathcal{J}_{k}^{(n+1)}\right]}, \\
k, n \in \mathbb{N}_{0}.
\end{aligned}$$
(2.23a)
(2.23b)

In [88, pp. 284 - 285], one finds the listing a FORTRAN 77 program that computes $\mathcal{J}_k^{(n)}$ using a single one-dimensional array.

Based on the explicit expression (2.22) for $\vartheta_2^{(n)}$, an alternative recursive scheme for $\mathscr{J}_k^{(n)}$ was derived in [92, Eq. (4.11)] and used for the prediction of unknown power series coefficients.

The iterated transformation $\mathscr{J}_k^{(n)}$ has similar properties as the theta algorithm from which it was derived. Both are very powerful as well as very versatile. $\mathscr{J}_k^{(n)}$ 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 (see for example [72, 88, 89, 91, 92] and references therein).

As discussed in Appendix B, the special case $\vartheta_2^{(n)} = \mathscr{J}_1^{(n)}$ of the iterated transformation $\mathscr{J}_k^{(n)}$ can be related to the *u* and *v* variants of Levin's general transformation [55, Eq. (22)] defined by Eq. (B.2). For Levin's *u* and *v* variants [55, Eqs. (59) and (68)], we use the notation [88, Eqs. (7.3-5) and (7.3-11)]:

$$u_{k}^{(n)}(\beta, S_{n}) = \mathscr{L}_{k}^{(n)}(\beta, S_{n}, (\beta + n)\Delta S_{n-1}), \qquad (2.24)$$

$$\nu_k^{(n)}(\boldsymbol{\beta}, \boldsymbol{s}_n) = \mathscr{L}_k^{(n)}(\boldsymbol{\beta}, \boldsymbol{S}_n, \Delta \boldsymbol{S}_{n-1}\Delta \boldsymbol{S}_n / [\Delta \boldsymbol{S}_{n-1} - \Delta \boldsymbol{S}_n]).$$
(2.25)

Equations (2.19), (B.8) and (B.12) imply (see also [88, Eq. (10.3-4)]):

$$\vartheta_2^{(n)} = u_2^{(n+1)}(\beta, S_{n+1}), \qquad (2.26)$$

$$= v_1^{(n+1)}(\beta, S_{n+1}), \qquad n \in \mathbb{N}_0, \quad \beta > 0.$$
(2.27)

3 Difference equations with respect to the transformation order

3.1 General Considerations

In this Section, we want to clarify the relationship between known generalizations of Wynn's epsilon and rho algorithm, and – more important – we also want to derive new generalizations. For that purpose, we pursue a novel approach and look at their recursions from the perspective of finite difference equations with respect to the transformation order k.

Our approach is based on the observation that the recursions (2.6b), (2.10b), (2.12b), and (2.14b) for Wynn's epsilon and rho algorithm and its special cases all possess the following general structure:

$$F_k^{(n)} = \left[T_{k+1}^{(n)} - T_{k-1}^{(n+1)}\right] \left[T_k^{(n+1)} - T_k^{(n)}\right], \qquad k, n \in \mathbb{N}_0.$$
(3.1)

The quantities $F_k^{(n)}$, which in general depend on both *k* and *n*, fully characterize the corresponding transformations. The algebraic properties of sequence transformations satisfying a recursion of the type of Eq. (3.1) had already been studied by Brezinski in his thesis [17, pp. 120 - 127] (see also [28, pp. 106 - 107]).

As shown later, many known variants of epsilon and rho can be classified according to the properties of $F_k^{(n)}$. This alone makes our subsequent analysis based on Eq. (3.1) useful. But it is our ultimate goal to construct new generalizations of epsilon and rho.

In principle, we could try to achieve our aim of constructing new transformations by simply choosing new and hopefully effective expressions for $F_k^{(n)}$ in Eq. (3.1). In combination with suitable initial conditions, this would produce recursive schemes for new sequence transformations. To the best of our knowledge, questions of that kind have not been treated in the literature yet. So – frankly speaking – we simply do not know how a practically useful $F_k^{(n)}$ should look like.

In order to get some help in this matter, we will make some specific assumptions about the dependence of the $F_k^{(n)}$ as functions of k and n. These assumptions will allow us to investigate whether and under which conditions the $F_k^{(n)}$ satisfy certain finite difference equations in the transformation order k. It will become clear later that our analysis of the resulting finite difference equations in k leads to some insight which ultimately makes it possible to construct new sequence transformations.

For an analysis of the *known* variants of epsilon and rho, the full generality of Eq. (3.1) is only needed in the case of the general form (2.10) of Wynn's rho algorithm with unspecified interpolation points $\{x_n\}$. In all other cases, the apparent *n*-dependence of the right-hand side of Eq. (3.1) cancels out and we only have to deal with a simpler, *n*-independent expression of the following general structure:

$$F_{k} = \left[T_{k+1}^{(n)} - T_{k-1}^{(n+1)}\right] \left[T_{k}^{(n+1)} - T_{k}^{(n)}\right], \qquad k, n \in \mathbb{N}_{0}.$$
(3.2)

In the case of the epsilon algorithm (2.6), we have $F_k = 1$, in the case of the standard form (2.12) of the rho algorithm, we have $F_k = k + 1$, and in the case of Osada's generalization (2.14), we have $F_k = k + \theta$.

3.2 First order difference equations

The simplest case $F_k = 1$ in Eq. (3.2), which corresponds to Wynn's epsilon algorithm (2.6), satisfies the following first order finite difference equation in *k*:

$$\Delta_k F_k = F_{k+1} - F_k = 0, \qquad k \in \mathbb{N}_0.$$
(3.3)

Equation (3.3) implies that the recursion (3.2) can also be expressed as follows:

$$\begin{bmatrix} T_{k+2}^{(n)} - T_k^{(n+1)} \end{bmatrix} \begin{bmatrix} T_{k+1}^{(n+1)} - T_{k+1}^{(n)} \end{bmatrix} - \begin{bmatrix} T_{k+1}^{(n)} - T_{k-1}^{(n+1)} \end{bmatrix} \begin{bmatrix} T_k^{(n+1)} - T_k^{(n)} \end{bmatrix} = 0.$$
 (3.4)

This reformulation of Eq. (3.2) does not look like a great achievement. It also appears to be a bad idea to use the more complicated recursion (3.4) instead of the much simpler recursion (3.2). However, the more complicated recursion (3.4) will help us to understand better certain features of the simpler recursion (3.2) and of the epsilon algorithm (2.6). In addition, the recursion (3.4) as well as related expressions occurring later open the way for the construction of new sequence transformations.

The first order finite difference equation $\Delta_m f(m) = f(m+1) - f(m) = 0$ with $m \in \mathbb{N}_0$ possesses the general solution f(m) = f(0). Thus, Eq. (3.3) implies $F_k = F_0$, and Eq. (3.2) can be rewritten as follows:

$$T_{k+1}^{(n)} = T_{k-1}^{(n+1)} + \frac{F_0}{T_k^{(n+1)} - T_k^{(n)}}, \qquad k, n \in \mathbb{N}_0.$$
(3.5)

If we choose $F_0 = 1$, we obtain Wynn's epsilon algorithm (2.6).

Alternatively, we could also assume that F_0 is a non-zero constant. By combining Eq. (3.5) with the epsilon-type initial conditions $T_{-1}^{(n)} = 0$ and $T_0^{(n)} = S_n$, we obtain $T_{2k}^{(n)} = \varepsilon_{2k}^{(n)}$ and $T_{2k+1}^{(n)} = F_0 \varepsilon_{2k+1}^{(n)}$. But only the transforms $T_{2k}^{(n)} = \varepsilon_{2k}^{(n)}$ with *even* subscripts provide approximations to the limit of the input sequence, whereas the transforms $T_{2k+1}^{(n)} = F_0 \varepsilon_{2k+1}^{(n)}$ with *odd* subscripts are only auxiliary quantities. Thus, the modified recursion (3.5) with $F_0 \neq 0$ does not produce anything new, and the epsilon algorithm remains invariant if we replace in Eq. (2.6b) $1/[\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}]$ by $F_0/[\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}]$. To the best of our knowledge, this invariance of the epsilon algorithm had not been observed before.

A similar invariance exists in the case of the general form (2.10) of Wynn's rho algorithm and its variants. If we replace the interpolation points $\{x_n\}$ by the scaled interpolation points $\{\alpha x_n\}$ with $\alpha > 0$, we obtain $\rho_{2k}^{(n)}(\alpha x_n) = \rho_{2k}^{(n)}(x_n)$ and $\rho_{2k+1}^{(n)}(\alpha x_n) = \alpha \rho_{2k+1}^{(n)}(x_n)$. This invariance can also be deduced from the determinantal representation for $\rho_{2k}^{(n)}$ [20, Theoreme 2.1.52 on p. 97].

Our assumption, that F_k satisfies the first order finite difference equation (3.3) in k and is therefore constant as a function of k, is apparently too restrictive to allow the construction of *useful* alternative transformations beyond Wynn's epsilon algorithm.

Let us now assume that the *n*-dependence of $F_k^{(n)}$ is such that the first order finite difference equation

$$\Delta_k F_k^{(n)} = F_{k+1}^{(n)} - F_k^{(n)} = 0, \qquad k, n \in \mathbb{N}_0,$$
(3.6)

is satisfied for all $n \in \mathbb{N}_0$. Then, the finite difference equation (3.6) implies $F_k^{(n)} = F_0^{(n)}$ and

$$T_{k+1}^{(n)} = T_{k-1}^{(n+1)} + \frac{F_0^{(n)}}{T_k^{(n+1)} - T_k^{(n)}}, \qquad k, n \in \mathbb{N}_0.$$
(3.7)

If we choose $F_0^{(n)} = x_{n+1} - x_n$ in Eq. (3.7), we obtain Brezinski's first generalization of the epsilon algorithm [18, p. 72], and if we choose $F_0^{(n)} = x_{n+k+1} - x_{n+k}$, we formally obtain Brezinski's second generalization [18, p. 78]. However, Brezinski's second generalization is only a special case of the recursion (3.7) if the original *k*-dependence of the interpolation points x_{n+k} is eliminated by forming the differences $\Delta x_{n+k} = x_{n+k+1} - x_{n+k}$.

By combining the recursion (3.7) with suitable initial conditions and suitable choices for $F_0^{(n)}$, we obtain new sequence transformations. Possible choices of the initial conditions will be be discussed in Section 3.4.

3.3 Second order difference equations

We have $F_k = k + 1$ in the case of the standard form (2.12) of Wynn's rho algorithm, and in the case of Osada's generalization (2.14) we have $F_k = k + \theta$. Thus, it looks like a natural idea to assume that F_k is linear in k, which means that F_k is annihilated by Δ_k^2 :

$$\Delta_k^2 F_k = F_{k+2} - 2F_{k+1} + F_k = 0, \qquad k \in \mathbb{N}_0.$$
(3.8)

The second order finite difference equation (3.8) is equivalent to the recursion

$$\begin{bmatrix} T_{k+3}^{(n)} - T_{k+1}^{(n+1)} \end{bmatrix} \begin{bmatrix} T_{k+2}^{(n+1)} - T_{k+2}^{(n)} \end{bmatrix} - 2 \begin{bmatrix} T_{k+2}^{(n)} - T_{k}^{(n+1)} \end{bmatrix} \begin{bmatrix} T_{k+1}^{(n+1)} - T_{k+1}^{(n)} \end{bmatrix} + \begin{bmatrix} T_{k+1}^{(n)} - T_{k-1}^{(n+1)} \end{bmatrix} \begin{bmatrix} T_{k}^{(n+1)} - T_{k}^{(n)} \end{bmatrix} = 0, \qquad k, n \in \mathbb{N}_{0},$$
(3.9)

which is even more complicated than the analogous recursion (3.4) based on the first order difference equation (3.3).

The second order finite difference equation $\Delta_m^2 f(m) = f(m+2) - 2f(m+1) + f(m) = 0$ with $m \in \mathbb{N}_0$ possesses the general solution f(m) = f(0) + m[f(1) - f(0)]. Thus, Eq. (3.8) implies $F_k = F_0 + k[F_1 - F_0]$, which means that Eq. (3.2) can be reformulated as follows:

$$T_{k+1}^{(n)} = T_{k-1}^{(n+1)} + \frac{F_0 + k[F_1 - F_0]}{T_k^{(n+1)} - T_k^{(n)}}, \qquad k, n \in \mathbb{N}_0.$$
(3.10)

This recursion contains several variants of Wynn's rho algorithm as special cases. If we choose $F_0 = 1$ and $F_1 = 2$, we obtain the standard form (2.12) of Wynn's rho algorithm, and if we choose $F_0 = \theta$ and $F_1 = \theta + 1$, we obtain Osada's variant (2.14) of the rho algorithm. Finally, $F_0 = F_1 \neq 0$ yields epsilon. Other choices for F_0 and F_1 are obviously possible, but to the best of our knowledge they have not been explored yet in the literature.

Our approach based on finite difference equations in the transformation order k was successful in the case of the variants of rho mentioned above, but the general form (2.10) of Wynn's rho algorithm with essentially arbitrary interpolation points $\{x_n\}$ remains elusive. In the case of essentially arbitrary interpolation points $\{x_n\}$, we cannot express the numerator $x_{n+k+1} - x_n$ of the ratio in Eq. (2.10b) as an *n*-independent F_k according to Eq. (3.2).

At least, we have to employ the more general expression (3.1) involving a general *n*-dependent $F_k^{(n)}$. But even this does not guarantee success. Of course, $F_k^{(n)} = x_{n+k+1} - x_n$ with

unspecified and essentially *arbitrary* interpolation points $\{x_n\}$ implies the finite difference equation $\Delta_k^m F_k^{(n)} = \Delta_k^m x_{n+k+1}$ in k. But to achieve any progress, we would have to make specific assumptions on the index dependence of the interpolation points $\{x_n\}$.

Therefore, let us now assume that the *n*-dependence of $F_k^{(n)}$ is such that

$$\Delta_k^2 F_k^{(n)} = F_{k+2}^{(n)} - 2F_{k+1}^{(n)} + F_k^{(n)} = 0, \qquad k \in \mathbb{N}_0,$$
(3.11)

is satisfied for arbitrary $n \in \mathbb{N}_0$. This yields the general solution $F_k^{(n)} = F_0^{(n)} + k[F_1^{(n)} - F_0^{(n)}]$, which implies that the recursion (3.10) can be generalized as follows:

$$T_{k+1}^{(n)} = T_{k-1}^{(n+1)} + \frac{F_0^{(n)} + k[F_1^{(n)} - F_0^{(n)}]}{T_k^{(n+1)} - T_k^{(n)}}, \qquad k, n \in \mathbb{N}_0.$$
(3.12)

By combining this recursion with suitable initial conditions, we obtain a whole class of new sequence transformations. Possible choices of the initial conditions are discussed in Section 3.4.

3.4 Initial conditions for the new transformation

Let us first analyze the recursion (3.4) which can be reformulated as follows:

$$T_{k+2}^{(n)} = T_k^{(n+1)} + \frac{\left[T_{k+1}^{(n)} - T_{k-1}^{(n+1)}\right] \left[T_k^{(n+1)} - T_k^{(n)}\right]}{T_{k+1}^{(n+1)} - T_{k+1}^{(n)}}.$$
(3.13)

We have to investigate for which values of $k \in \mathbb{N}_0$ this recursion can hold, and how its initial conditions could or should be chosen.

It is an obvious idea to choose the initial conditions according to $T_{-1}^{(n)} = 0$ and $T_0^{(n)} = S_n$ as in the case of epsilon. However, these assumptions do not suffice here. Setting k = -1 in Eq. (3.13) yields:

$$T_{1}^{(n)} = T_{-1}^{(n+1)} + \frac{\left[T_{0}^{(n)} - T_{-2}^{(n+1)}\right] \left[T_{-1}^{(n+1)} - T_{-1}^{(n)}\right]}{T_{0}^{(n+1)} - T_{0}^{(n)}}.$$
(3.14)

The numerator on the right-hand side contains the undefined quantity $T_{-2}^{(n+1)}$ and the undefined finite difference $\Delta T_{-1}^{(n)} = T_{-1}^{(n+1)} - T_{-1}^{(n)}$. To remove these ambiguities, we could for example assume $\Delta T_{-1}^{(n)} = T_{-1}^{(n+1)} - T_{-1}^{(n)} = 0$ and $T_{-2}^{(n+1)}[T_{-1}^{(n+1)} - T_{-1}^{(n)}] = -1$. But in our opinion it would be simpler and more natural to use the recursion (3.13) in combination with suitable initial conditions only for $k \ge 0$.

If we set k = 0 in Eq. (3.13) and use the epsilon initial conditions $T_{-1}^{(n)} = 0$, $T_0^{(n)} = S_n$, and $T_1^{(n)} = 1/[T_0^{(n+1)} - T_0^{(n)}]$, we obtain

$$T_2^{(n)} = T_0^{(n+1)} + \frac{1}{T_1^{(n+1)} - T_1^{(n)}}.$$
(3.15)

Comparison with Eq. (2.6b) shows that $T_2^{(n)}$ is nothing but $\varepsilon_2^{(n)}$ in disguise. Next, we set k = 1 in Eq. (3.13):

$$T_3^{(n)} = T_1^{(n+1)} + \frac{\left[T_2^{(n)} - T_0^{(n+1)}\right] \left[T_1^{(n+1)} - T_1^{(n)}\right]}{T_2^{(n+1)} - T_2^{(n)}}.$$
(3.16)

At first sight, this looks like a new expression $T_3^{(n)} \neq \varepsilon_3^{(n)}$. Unfortunately, Eq. (3.15) implies $T_2^{(n)} - T_0^{(n+1)} = 1/[T_1^{(n+1)} - T_1^{(n)}]$. Thus, we obtain $T_3^{(n)} = \varepsilon_3^{(n)}$, and with the help of complete induction in k we deduce $T_k^{(n)} = \varepsilon_k^{(n)}$ for $k \ge 3$, or actually for all $k \in \mathbb{N}_0$. These considerations show that the recursion (3.13) produces nothing new if we use it in combination with the epsilon initial conditions $T_{-1}^{(n)} = 0$, $T_0^{(n)} = S_n$, and $T_1^{(n)} = 1/[T_0^{(n+1)} - T_0^{(n)}]$. We will now discuss the choice of *alternative* initial conditions for the recursion (3.12),

We will now discuss the choice of *alternative* initial conditions for the recursion (3.12), which is based on the assumption that $F_k^{(n)}$ satisfies the second order finite difference equation (3.11). This is a crucial step, and it is also the point where our approach becomes experimental.

We choose parts of the initial values of the recursion (3.9) as in Wynn's epsilon algorithm:

$$T_{-1}^{(n)} = 0, \quad T_0^{(n)} = S_n, \quad T_1^{(n)} = \frac{1}{\Delta S_n}, \qquad n \in \mathbb{N}_0.$$
 (3.17)

With these initial conditions, epsilon and rho are recovered by choosing $T_2^{(n)} = \varepsilon_2^{(n)}$ and $T_2^{(n)} = \rho_2^{(n)}$, respectively.

If we want to employ the recursion (3.9), we first have to make a choice about the initial value $F_1^{(n)}$. Equation (3.1) implies $F_1^{(n)} = [T_2^{(n)} - T_0^{(n+1)}][T_1^{(n+1)} - T_1^{(n)}]$. If $T_{-1}^{(n)}$, $T_0^{(n)}$, and $T_1^{(n)}$ are chosen according to Eq. (3.17), we only need one further choice for $T_2^{(n)}$ to fix $F_1^{(n)}$.

It is a relatively natural idea to choose $T_2^{(n)}$ in such a way that it corresponds to the special case of a sequence transformation with low transformation order. If we want the resulting new transformation to be more versatile than either epsilon or rho, it makes sense to choose a transformation which is known to accelerate both linear and logarithmic convergence effectively. Obvious candidates would be the spacial case $\vartheta_2^{(n)}$ of Brezinski's theta algorithm discussed in Section 2.3, or suitable variants of Levin's transformation discussed in Appendices B.2 and B.3.

There is another decision, which we have to make. Should the expression for $T_2^{(n)}$ depend on *n* only *implicitly* via the input data $\{S_n\}$, or can it depend on *n* also *explicitly* (examples of low order transformations of that kind can be found in [89, Section 3]). We think that it would be more in agreement with the spirit of the other initial conditions (3.17) if we require that $T_2^{(n)}$ depends on *n* only *implicitly* via the input data.

Under these assumptions, it looks like an obvious idea to identify $T_2^{(n)}$ either with Brezinski's theta transformation $\vartheta_2^{(n)}$ given by Eq. (2.19) or with the explicit expressions for the Levin *u* and *v* transformations $u_2^{(n)}(\beta, S_n)$ and $v_1^{(n)}(\beta, S_n)$ given by Eqs. (2.26) and (2.27).

We checked the performance of the resulting algorithms numerically. For $T_2^{(n)} = \vartheta_2^{(n)} = u_2^{(n+1)}(\beta, S_{n+1}) = v_1^{(n+1)}(\beta, S_{n+1})$ (compare Eqs. (2.26) and (2.27)), we obtained consistently good results, but our results for $T_2^{(n)} = u_2^{(n)}(\beta, S_n) = v_1^{(n)}(\beta, S_n)$ (compare Eqs. (B.8) and (B.12)) were less good. Thus, we will exclusively use the following non-epsilon initial

condition:

$$T_{2}^{(n)} = \vartheta_{2}^{(n)} = u_{2}^{(n+1)}(\beta, S_{n+1}) = v_{1}^{(n+1)}(\beta, S_{n+1})$$

= $S_{n+1} - \frac{[\Delta^{2}S_{n+1}][\Delta S_{n}][\Delta S_{n+1}]}{[\Delta S_{n+2}][\Delta^{2}S_{n}] - [\Delta S_{n}][\Delta^{2}S_{n+1}]}, \quad n \in \mathbb{N}_{0}.$ (3.18)

Then, Eq. (3.1) implies

$$F_0^{(n)} = 1, \quad F_1^{(n)} = \frac{\left[\Delta^2 T_0^{(n)}\right] \left[\Delta^2 T_0^{(n+1)}\right]}{\left[\Delta T_0^{(n+2)}\right] \left[\Delta^2 T_0^{(n)}\right] - \left[\Delta T_0^{(n)}\right] \left[\Delta^2 T_0^{(n+1)}\right]}$$
(3.19)

and we obtain the following new recursive scheme:

$$\tilde{T}_0^{(n)} = S_n, \tag{3.20a}$$

$$\tilde{T}_{1}^{(n)} = \frac{1}{\tilde{T}_{0}^{(n+1)} - \tilde{T}_{0}^{(n)}},$$
(3.20b)

$$\tilde{T}_{2}^{(n)} = \tilde{T}_{0}^{(n+1)} - \frac{\left[\Delta \tilde{T}_{0}^{(n)}\right] \left[\Delta \tilde{T}_{0}^{(n+1)}\right] \left[\Delta^{2} \tilde{T}_{0}^{(n+1)}\right]}{\left[\Delta \tilde{T}_{0}^{(n+2)}\right] \left[\Delta^{2} \tilde{T}_{0}^{(n)}\right] - \left[\Delta \tilde{T}_{0}^{(n)}\right] \left[\Delta^{2} \tilde{T}_{0}^{(n+1)}\right]},$$
(3.20c)

$$F_{1}^{(n)} = \frac{\left[\Delta^{2}\tilde{T}_{0}^{(n)}\right]\left[\Delta^{2}\tilde{T}_{0}^{(n+1)}\right]}{\left[\Delta\tilde{T}_{0}^{(n+2)}\right]\left[\Delta^{2}\tilde{T}_{0}^{(n)}\right] - \left[\Delta\tilde{T}_{0}^{(n)}\right]\left[\Delta^{2}\tilde{T}_{0}^{(n+1)}\right]},$$
(3.20d)

$$\tilde{T}_{k+1}^{(n)} = \tilde{T}_{k-1}^{(n+1)} + \frac{1-k+kF_1^{(n)}}{\tilde{T}_k^{(n+1)} - \tilde{T}_k^{(n)}}, \qquad k = 2, 3, \dots, \qquad n \in \mathbb{N}_0.$$
(3.20e)

In Eq. (3.20), we wrote \tilde{T} instead of *T* in order to distinguish our new algorithm from others mentioned before. The performance of our new algorithm (3.20) will be studied in detail in the following Section 4.

4 Numerical examples

In this section, we apply our new algorithm (3.20) to some linearly and logarithmically convergent sequences and also to some divergent series. We compare the numerical results of our new algorithm with those obtained by applying Wynn's epsilon and rho algorithms (2.6) and (2.12), Osada's generalized rho algorithm (2.14), Brezinski's theta algorithm (2.18) and the iteration (2.23) of $\vartheta_2^{(n)}$. All the numerical computation are obtained with the help of MATLAB 7.0 in double precision (15 decimal digits).

4.1 Asymptotic model sequences

In this Section, we want to analyze the numerical performance of our new sequence transformation (3.20). As input data, we use some model sequences which provide reasonably good approximations to the elements of numerous practically relevant sequences in the limit of large indices. Essentially the same model sequences had been used by Sidi in [72, Eqs. (1.1) - (1.3)] and in [73, Definition 15.3.2 on p. 285], and by Weniger [93, Section IV]: 1. Logarithmically convergent model sequence

$$S_n = S + \sum_{j=0}^{\infty} c_j n^{\eta-j}, \qquad c_0 \neq 0, \quad n \in \mathbb{N}_0.$$
 (4.1)

2. Linearly convergent model sequence

$$S_n = S + \xi^n \sum_{j=0}^{\infty} c_j n^{\eta-j}, \qquad c_0 \neq 0, \quad n \in \mathbb{N}_0.$$
 (4.2)

3. Hyperlinearly convergent model sequence

$$S_n = S + \frac{\xi^n}{(n!)^r} \sum_{j=0}^{\infty} c_j n^{\eta-j}, \qquad c_0 \neq 0, \quad r \in \mathbb{R}, \quad n \in \mathbb{N}_0.$$
(4.3)

The series expansions Eqs. (4.1) – (4.3) are to be interpreted as purely *formal* expansions, i.e., we do not tacitly assume that they converge. It is actually more realistic to assume that they are only asymptotic to S_n as $n \to \infty$. There are, however, restrictions on the parameters η and ξ if we require that the sequences $\{S_n\}$ defined by the series expansions Eqs. (4.1) – (4.3) are able to represent something finite.

The sequence $\{S_n\}$ defined by Eq. (4.1) can only converge to its limit *S* if $\eta < 0$ holds. For $\eta > 0$, Sidi [72, Text following Eq. (1.1)] calls *S* the *antilimit* of this sequence. While this terminology is very useful in the case of divergent, but summable series, it is highly questionable here. The divergence of this sequence for $\eta > 0$ is genuine, and the normally used summation techniques are not able to produce anything finite. Thus, the terminology *antilimit* does not make sense here.

The sequence $\{S_n\}$ defined by Eq. (4.2) converges for all $\eta \in \mathbb{R}$ linearly to its limit *S* provided that $|\xi| < 1$ holds. For $|\xi| > 1$, this sequence diverges, but it should normally be summable to *S* for all ξ belonging to the cut complex plane $\mathbb{C} \setminus [1, \infty)$.

The most convenient situation occurs if the sequence elements S_n satisfy Eq. (4.3). Then, this sequence converges for all $\xi, \eta \in \mathbb{R}$ hyperlinearly to its limit *S*. In Eq. (4.3), the restriction $r \in \mathbb{R}_+$ is essential, because for r < 0, we would obtain a sequence which diverges (hyper)factorially for all $\xi \neq 0$. Divergent sequences of that kind can according to experience often be summed to their generalized limits *S* for all $\xi \in \mathbb{C} \setminus [0, \infty)$, but a rigorous theoretical analysis of such a summation process is normally extremely difficult (compare the rigorous theoretical analysis of the summation of a comparatively simple special case in [13] and references therein).

4.2 Linearly convergent sequences

In this Subsection, we apply our new algorithm to some linearly convergent alternating and monotone series, which are special cases of the model sequence (4.1). The numerical results obtained by our new algorithm (3.20), Wynn's epsilon algorithm (2.6), Brezinski's theta algorithm (2.18) and the iteration (2.23) of $\vartheta_2^{(n)}$ are presented in Tables 4.1 and 4.2.

In the captions of the following Tables, [x] denotes the *integral part* of *x*, which is the *largest* integer *n* satisfying $n \le x$.

Example 4.1: We consider the alternating partial sums

$$S_n = \sum_{k=0}^n \frac{(-1)^k}{k+1}, \qquad n \in \mathbb{N}_0,$$
(4.4)

n	$ S_n - S $	$\left \tilde{T}_{2 (n-1)/2 }^{(n-1-2\lfloor (n-1)/2 \rfloor)} - S \right $	$\left \varepsilon_{2\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)} - S\right $	$\left \vartheta_{2\lfloor n/3\rfloor}^{(n-3\lfloor n/3\rfloor)}-S\right $	$\left \mathcal{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right $
	Eq. (4.4)	Eq. (3.20)	Eq. (2.6)	Eq. (2.18)	Eq. (2.23)
7	0.059	6.768×10^{-7}	1.437×10^{-6}	5.702×10^{-7}	1.527×10^{-8}
8	0.052	3.485×10^{-8}	1.518×10^{-7}	1.961×10^{-7}	7.793×10^{-9}
9	0.048	5.907×10^{-9}	3.807×10^{-8}	8.881×10^{-10}	6.034×10^{-10}
10	0.043	1.920×10^{-9}	4.402×10^{-9}	2.764×10^{-10}	2.115×10^{-10}
11	0.040	8.728×10^{-11}	1.042×10^{-9}	9.280×10^{-11}	7.530×10^{-11}
12	0.037	4.244×10^{-11}	1.282×10^{-10}	1.171×10^{-13}	4.954×10^{-13}
13	0.034	1.396×10^{-11}	2.909×10^{-11}	1.665×10^{-14}	3.331×10^{-14}
14	0.032	3.936×10^{-13}	3.745×10^{-12}	1.266×10^{-14}	2.331×10^{-15}

Table 4.1 Numerical results of example 4.1

Table 4.2 Numerical results of example 4.2

п	$ S_n - S $	$\left \tilde{T}_{2 \mid (n-1)/2 \mid}^{(n-1-2 \lfloor (n-1)/2 \rfloor)} - S \right $	$\left \varepsilon_{2\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)} - S \right $	$\left \vartheta_{2\left\lfloor n/3 ight floor}^{\left(n-3\left\lfloor n/3 ight floor}-S ight $	$\left \mathcal{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right $
	Eq. (4.6)	Eq. (3.20)	Eq. (2.6)	Eq. (2.18)	Eq. (2.23)
13	9.657×10^{-3}	7.687×10^{-4}	3.637×10^{-6}	3.533×10^{-6}	9.972×10^{-10}
14	7.312×10^{-3}	1.226×10^{-4}	1.272×10^{-6}	3.560×10^{-6}	2.092×10^{-10}
15	5.552×10^{-3}	3.558×10^{-4}	5.260×10^{-7}	3.561×10^{-6}	2.026×10^{-9}
16	4.228×10^{-3}	4.880×10^{-5}	1.860×10^{-7}	3.585×10^{-6}	2.479×10^{-10}
17	3.227×10^{-3}	1.608×10^{-5}	7.597×10^{-8}	3.573×10^{-6}	6.144×10^{-11}
18	2.469×10^{-3}	1.990×10^{-5}	2.769×10^{-8}	3.582×10^{-6}	3.903×10^{-11}
19	1.892×10^{-3}	8.434×10^{-6}	1.025×10^{-8}	1.837×10^{-6}	5.445×10^{-11}
20	1.453×10^{-3}	4.816×10^{-6}	5.256×10^{-9}	5.225×10^{-9}	4.459×10^{-11}

which converge to $S = \ln(2)$. The Boole summation formula [59, Eq. (24.17.1)] yields

$$S_n - \ln(2) \sim \frac{(-1)^{n-1}}{2} \left\{ \frac{1}{n+1} + O(n^{-2}) \right\}, \qquad n \to \infty.$$
 (4.5)

This truncated asymptotic expansion is a special case of the model sequence (4.2) with $\xi = -1$ and $\eta = -1$.

Example 4.2: The linearly convergent monotone sequence

$$S_n = \frac{4}{5} \sum_{k=0}^n \frac{(4/5)^k}{k+1}, \qquad n \in \mathbb{N}_0,$$
(4.6)

converges to $S = \ln(5)$ as $n \to \infty$. As shown by Sidi [73, p. 84], S_n possesses the asymptotic expansion

$$S_n - \ln(5) \sim \frac{(4/5)^n}{n} \left\{ -4 + O(n^{-2}) \right\}, \qquad n \to \infty,$$
 (4.7)

which is a special case of the model sequence (4.2) with $\xi = 4/5$ and $\eta = -1$.

4.3 Logarithmically convergent sequences

First, we consider a logarithmically convergent sequence of the type of the model sequence (2.13) with integral decay parameter θ . In Table 4.3, we present the numerical results obtained by applying our new algorithm (3.20), the standard form (2.12) of Wynn's rho algorithm, Brezinski's theta algorithm (2.18), and the iteration (2.23) of $\vartheta_2^{(n)}$. Other logarithmically convergent sequences with non-integral decay parameters θ will be discussed later.

п	$ S_n - S $	$\left \tilde{T}_{2\lfloor (n-1)/2\rfloor}^{(n-1-2\lfloor (n-1)/2\rfloor)}-S\right $	$\left ho_{2\left\lfloor n/2 ight floor}^{\left(n-2\left\lfloor n/2 ight floor} ight)}-S ight $	$\left \vartheta_{2\left\lfloor n/3 ight floor}^{\left(n-3\left\lfloor n/3 ight floor}-S ight $	$\left \mathcal{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right $
	Eq. (4.8)	Eq. (3.20)	Eq. (2.12)	Eq. (2.18)	Eq. (2.23)
3	0.120	4.051×10^{-4}	2.942×10^{-4}	4.051×10^{-4}	4.051×10^{-4}
4	0.097	3.190×10^{-4}	6.774×10^{-5}	3.190×10^{-4}	3.190×10^{-4}
5	0.081	6.518×10^{-4}	7.156×10^{-6}	1.875×10^{-4}	1.875×10^{-4}
6	0.070	2.724×10^{-5}	8.286×10^{-8}	2.391×10^{-4}	2.393×10^{-4}
7	0.061	1.521×10^{-8}	5.091×10^{-9}	2.221×10^{-5}	2.238×10^{-5}
8	0.055	1.188×10^{-8}	1.870×10^{-9}	4.735×10^{-6}	4.822×10^{-6}
9	0.049	5.295×10^{-9}	6.288×10^{-10}	2.316×10^{-7}	1.974×10^{-7}
10	0.045	6.931×10^{-10}	1.289×10^{-11}	4.116×10^{-8}	7.269×10^{-9}

Table 4.3 Numerical results of example 4.3

Example 4.3: We consider the logarithmically convergent sequence

$$S_n = 1 + \sum_{k=1}^n \left\{ \frac{1}{k+1} + \log\left(\frac{k}{k+1}\right) \right\}, \qquad n \in \mathbb{N},$$
(4.8)

which converges to $S = 0.577215664901532\cdots$ (Euler's constant).

The Euler-Maclaurin formula (see for example [59, Eq. (2.10.1)]) yields:

$$S_{n-1} = \sum_{k=1}^{n} \frac{1}{k} - \log(n) \sim S + n^{-1} \left(\frac{1}{2} + \sum_{j=1}^{\infty} \frac{B_{2j}}{2j} n^{-2j} \right), \qquad n \to \infty,$$
(4.9)

where B_n is a Bernoulli number [59, Eq. (24.2.1)].

Next, we consider logarithmically convergent sequences of the form of Eq. (4.1) with non-integral decay θ . In Table 4.4, we present the numerical results for the test problem (4.10) obtained by our new algorithm (3.20), Osada's generalized rho algorithm (2.14) with $\theta = 1/2$, Brezinski's theta algorithm (2.18) and the iteration (2.23) of $\vartheta_2^{(n)}$.

Example 4.4: A very useful test problem is the series expansion for the so-called lemniscate constant *A* [81, Theorem 5]:

$$A = \frac{[\Gamma(1/4)]^2}{4(2\pi)^{1/2}} = \sum_{m=0}^{\infty} \frac{(2m-1)!!}{(2m)!!} \frac{1}{4m+1}.$$
 (4.10)

Standard asymptotic techniques show that the terms (2m-1)!!/[(2m)!!(4m+1)] of this series decay like $m^{-3/2}$ as $m \to \infty$. This implies that the remainders

$$R_n = S_n - S = \sum_{m=n+1}^{\infty} \frac{(2m-1)!!}{(2m)!!} \frac{1}{4m+1}$$
(4.11)

decay like $n^{-1/2}$ as $n \to \infty$. Consequently, the series expansion (4.10) constitutes an extremely challenging convergence acceleration problem. Todd [81, p. 14] stated in 1975 that this series expansion is of no practical use for the computation of *A*, which is certainly true if no convergence acceleration techniques are available. In 1979, the series expansion (4.10) was used by Smith and Ford [74, Entry 13 of Table 6.1] to test the ability of sequence transformations of accelerating logarithmic convergence. They observed that the standard form (2.12) of Wynn's rho algorithm fails to accelerate the convergence of this series [74, p. 235] which is in agreements with Osada's later convergence analysis [60, Theorem 3.2]. The series expansion (4.10) was also extensively used by Weniger [88, Tables 14-2 - 14-4] as a test case.

п	$ S_n - S $	$\left \tilde{T}_{2\lfloor (n-1)/2\rfloor}^{(n-1-2\lfloor (n-1)/2\rfloor)}-S\right $	$\left \bar{\rho}_{2 n/2 }^{(n-2\lfloor n/2\rfloor)} - S \right $	$\left \vartheta_{2\lfloor n/3\rfloor}^{(n-3\lfloor n/3\rfloor)}-S\right $	$\left \mathscr{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right $
	Eq. (4.11)	Eq. (3.20)	Eq. (2.14), $\theta = 1/2$	Eq. (2.18)	Eq. (2.23)
14	0.073	1.029×10^{-8}	8.637×10^{-12}	8.733×10^{-10}	2.680×10^{-9}
15	0.071	1.201×10^{-10}	1.038×10^{-12}	5.325×10^{-10}	2.565×10^{-9}
16	0.069	5.704×10^{-11}	2.517×10^{-12}	5.542×10^{-10}	1.921×10^{-9}
17	0.067	1.081×10^{-10}	9.550×10^{-13}	1.299×10^{-9}	9.512×10^{-9}
18	0.065	1.606×10^{-11}	1.384×10^{-11}	5.174×10^{-10}	2.457×10^{-9}
19	0.063	1.333×10^{-10}	6.473×10^{-13}	1.086×10^{-9}	7.667×10^{-9}
20	0.062	1.583×10^{-11}	3.970×10^{-13}	1.614×10^{-6}	7.311×10^{-8}
21	0.060	1.591×10^{-12}	6.120×10^{-13}	2.152×10^{-7}	1.540×10^{-8}

Table 4.4 Numerical results of example 4.4

Table 4.5 Numerical results of example 4.5

п	$ S_n - S $	$\left \tilde{T}_{2 (n-1)/2 }^{(n-1-2\lfloor (n-1)/2 \rfloor)} - S \right $	$\left ar{oldsymbol{ ho}}_{2\lfloor n/2 floor}^{(n-2\lfloor n/2 floor)}-S ight $	$\left \vartheta_{2\lfloor n/3 floor}^{(n-3\lfloor n/3 floor} - S \right $	$\left \mathcal{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right $
	Eq. (4.12)	Eq. (3.20)	Eq. (2.14), $\theta = 1/2$	Eq. (2.18)	Eq. (2.23)
14	0.149	4.688×10^{-9}	3.580×10^{-10}	4.073×10^{-5}	1.149×10^{-7}
15	0.144	3.321×10^{-9}	1.266×10^{-10}	4.362×10^{-5}	1.068×10^{-8}
16	0.139	1.443×10^{-8}	2.067×10^{-10}	2.654×10^{-5}	8.333×10^{-10}
17	0.135	1.086×10^{-9}	1.338×10^{-10}	5.316×10^{-8}	4.021×10^{-9}
18	0.131	3.993×10^{-9}	3.329×10^{-11}	8.259×10^{-8}	2.607×10^{-9}
19	0.128	4.042×10^{-10}	8.087×10^{-11}	5.279×10^{-8}	7.819×10^{-10}
20	0.125	2.013×10^{-9}	6.629×10^{-11}	5.270×10^{-8}	1.851×10^{-8}
21	0.122	1.075×10^{-11}	8.181×10^{-11}	5.275×10^{-8}	1.858×10^{-8}

Example 4.5: The series expansion (A.10) of 1/z in terms of reduced Bessel functions, whose basic properties are reviewed in Appendix A, is a challenging test problem for the ability of a sequence transformation to accelerate the convergence of a logarithmically convergent sequence with a non-integral decay parameter.

We consider the sequence of partial sum of the series (A.10) with z = 1,

$$S_n = \sum_{m=0}^n \hat{k}_{m-1/2}(1) / [2^m m!], \qquad (4.12)$$

which corresponds to a special case of the model sequence (4.1) with $\eta = -1/2$. In Table 4.5, we present the numerical results for the test problem (4.12) obtained by our new algorithm (3.20), Osada's generalized rho algorithm (2.14) with $\theta = 1/2$, Brezinski's theta algorithm (2.18) and the iteration (2.23) of $\vartheta_2^{(n)}$.

Our numerical Examples 4.3 - 4.5 show that our new algorithm is apparently able to accelerate the convergence of logarithmically convergent sequences of the type of (2.13) *without* having to know the value of the decay parameter θ explicitly, as it is necessary in the case of Osada's variant (2.14) of the rho algorithm.

4.4 Divergent series

In this Section, we apply our new algorithm for the summation of the factorially divergent Euler series. Since the early days of calculus, divergent series have been a highly controversial topic in mathematics [33, 41, 83], and to some extend they still are (see for example [95, Appendix D] and references therein).

The exponential integral [59, Eq. (6.2.1)]

$$E_1(z) = \int_z^\infty \frac{\exp(-t)}{t} dt$$
, (4.13)

possesses the asymptotic expansion [59, Eq. (6.12.1)]

$$ze^{z}E_{1}(z) \sim \sum_{m=0}^{\infty} \frac{(-1)^{m}m!}{z^{m}} = {}_{2}F_{0}(1,1;-1/z), \qquad z \to \infty.$$
 (4.14)

The exponential integral can be expressed as a Stieltjes integral [59, Eq. (6.7.1)],

$$e^{z}E_{1}(z) = \int_{0}^{\infty} \frac{\exp(-t)dt}{z+t} = \frac{1}{z} \int_{0}^{\infty} \frac{\exp(-t)dt}{1+t/z},$$
(4.15)

which implies that the divergent inverse power series (4.14) is a Stieltjes series.

Asymptotic series as $z \to \infty$ involving a factorially divergent generalized hypergeometric series ${}_2F_0$ occur also among other special functions. Examples are the asymptotic expansion of the modified Bessel function $K_v(z)$ of the second kind [59, Eq. (10.40.2)], or the asymptotic expansion of the Whittaker function $W_{\kappa,\mu}(z)$ of the second kind [59, Eq. (13.19.3)]. Similar divergent series occur also in statistics, as discussed in a book by Bowman and Shenton [15].

If we replace in Eq. (4.14) *z* by 1/z, we obtain the so-called Euler series, which had already been studied by Euler (see for example the books by Bromwich [32, pp. 323 - 324] and Hardy [50, pp. 26 - 29] or the articles by Barbeau [3] and Barbeau and Leah [4]). For $|\arg(z)| < \pi$, the Euler series is the asymptotic series of the Euler integral:

$$\mathscr{E}(z) = \int_0^\infty \frac{\mathrm{e}^{-t}}{1+zt} \,\mathrm{d}t \,\sim\, \sum_{\nu=0}^\infty \,(-1)^\nu \,\nu! \, z^\nu \,=\, _2F_0(1,1;-z)\,, \qquad z\to 0\,. \tag{4.16}$$

The Euler series is the most simple prototype of the factorially divergent perturbation series that occur abundantly in quantum physics. Already Dyson [40] had argued that perturbation expansions in quantum electrodynamics must diverge factorially. Around 1970, Bender and Wu [6, 7, 8] showed in their seminal work on anharmonic oscillators that factorially divergent perturbation expansions occur in nonrelativistic quantum mechanics. Later, it was found that factorially divergent perturbation expansions are actually the rule in quantum physics rather than the exception (see for example the articles by Fischer [44, Table 1] and Suslov [78], or the articles reprinted in the book by Le Guillou and Zinn-Justin [54]). Applications of factorially divergent series in optics are discussed in a recent review by Borghi [12].

The Euler integral $\mathscr{E}(z)$ is a Stieltjes function. Thus, the corresponding Euler series ${}_{2}F_{0}(1,1;-z)$ is its associated Stieltjes series (see for example [2, Chapter 5]). This Stieltjes property guarantees the convergence of certain subsequences of the Padé table of ${}_{2}F_{0}(1,1;-z)$ to the Euler integral (see for example [2, Chapter 5.2] or the discussion in [13]).

It has been shown in many calculations that sequence transformations are principal tools that can accomplish an efficient summation of the factorially divergent expansions of the type of the Euler series (see for example [13] and references therein). However, in the case of most sequence transformations, no rigorous theoretical convergence proofs are known (this applies also to Padé approximants if the series to be transformed is not Stieltjes). An exception is the delta transformation [88, Eq. (8.4-4)] of the Euler series, whose convergence to the Euler integral for all $z \in \mathbb{C} \setminus [0, \infty)$ was proved rigorously in [13].

п	$ S_n - S $ Eq. (4.17), z=3	$\begin{vmatrix} \tilde{T}_{2\lfloor (n-1)/2 \rfloor}^{(n-1-2\lfloor (n-1)/2 \rfloor)} - S \end{vmatrix}$ Eq. (3.20)	$\begin{vmatrix} \varepsilon_{2\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)} - S \end{vmatrix}$ Eq. (2.6)	$ \begin{vmatrix} \vartheta_{2\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \end{vmatrix} $ Eq. (2.18)	$\left \begin{array}{c} \mathcal{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right \\ \text{Eq. (2.23)} \end{array} \right $
14	1.504×10^{4}	2.587×10^{-8}	9.326×10^{-7}	5.357×10^{-11}	4.735×10^{-11}
15	7.609×10^{4}	3.287×10^{-9}	7.006×10^{-7}	1.379×10^{-11}	6.865×10^{-12}
16	4.100×10^{5}	1.568×10^{-9}	2.877×10^{-7}	4.047×10^{-11}	6.424×10^{-11}
17	2.344×10^{6}	3.844×10^{-11}	2.192×10^{-7}	3.737×10^{-10}	3.744×10^{-11}
18	1.418×10^{7}	8.860×10^{-9}	9.445×10^{-8}	4.069×10^{-11}	1.258×10^{-12}
19	9.048×10^{7}	2.204×10^{-9}	7.289×10^{-8}	6.707×10^{-11}	2.000×10^{-10}
20	6.073×10^{8}	4.265×10^{-9}	3.272×10^{-8}	3.673×10^{-13}	1.386×10^{-12}
21	4.277×10^{9}	2.101×10^{-10}	2.552×10^{-8}	9.726×10^{-14}	1.785×10^{-12}

Table 4.6 Summation of the asymptotic series ${}_2F_0(1,1;-1/z) = ze^z E_1(z)$ for z = 3

Table 4.7 Summation of the asymptotic series ${}_2F_0(1,1;-1/z) = ze^z E_1(z)$ for z = 1/2

п	$ S_n - S $	$\left \tilde{T}_{2\lfloor (n-1)/2 \rfloor}^{(n-1-2\lfloor (n-1)/2 \rfloor)} - S \right $	$\left \varepsilon_{2\lfloor n/2 \rfloor}^{(n-2\lfloor n/2 \rfloor)} - S \right $	$\left \vartheta_{2\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S\right $	$\left \mathcal{J}_{\lfloor n/3 \rfloor}^{(n-3\lfloor n/3 \rfloor)} - S \right $
	Eq. (4.17), z=1/2	Eq. (3.20)	Eq. (2.6)	Eq. (2.18)	Eq. (2.23)
14	1.379×10^{15}	3.012×10^{-4}	2.065×10^{-3}	3.963×10^{-5}	1.862×10^{-5}
15	4.147×10^{16}	4.489×10^{-5}	3.346×10^{-3}	4.578×10^{-7}	1.052×10^{-6}
16	1.330×10^{18}	1.498×10^{-5}	1.257×10^{-3}	1.314×10^{-7}	4.844×10^{-7}
17	4.529×10 ¹⁹	1.364×10^{-6}	1.987×10^{-3}	4.963×10^{-7}	2.710×10^{-7}
18	1.633×10^{21}	7.763×10^{-6}	7.876×10^{-4}	4.044×10^{-7}	2.207×10^{-6}
19	6.214×10^{22}	6.418×10^{-6}	1.218×10^{-3}	1.425×10^{-7}	4.204×10^{-7}
20	2.489×10^{24}	2.846×10^{-6}	5.052×10^{-4}	8.537×10^{-8}	2.591×10^{-7}
21	1.047×10^{26}	3.780×10^{-6}	7.662×10^{-4}	3.127×10^{-8}	3.538×10^{-7}

In the following Tables 4.6 and 4.7, we use as input data the partial sums

$$S_n = \sum_{m=0}^n (-1)^m m! z^{-m}$$
(4.17)

of the factorially divergent asymptotic series (4.14) for the exponential integral $E_1(z)$. We present the summation results obtained for z = 3 and z = 1/2, respectively, by our new algorithm (3.20), Wynn's epsilon algorithm (2.6), Brezinski's theta algorithm (2.18), and the iteration (2.23) of $\vartheta_2^{(n)}$.

5 Conclusions and discussions

Starting from the known recursion relations of Wynn's epsilon and rho algorithm or of Osada's generalized rho algorithm, we constructed a new convergence acceleration algorithm (3.20) which is – as shown in our numerical examples in Section 4 – not only successful in the case of linearly convergent sequences, but works also in the case of many logarithmically convergent sequences. Our numerical results also showed that our new transformations sums factorially divergent series. Thus, our new transformation (3.20) is clearly more versatile than either epsilon or rho, having similar properties as Brezinski's theta algorithm (2.18) or the iteration (2.23) of $\vartheta_2^{(n)}$.

For the derivation of our new algorithm (3.20) in Section 3, we pursued a novel approach. We analyzed the finite difference equations with respect to the transformation order, which the known recurrence formulas of Wynn's epsilon and rho algorithms or of Osada's generalized rho algorithm satisfy. This approach yielded a generalized recursive scheme (3.12)

which contains the known recursions of Wynn's epsilon and rho algorithms and Osada's rho algorithm as special cases.

To complete the derivation of our new algorithm (3.20), we only had to choose appropriate initial conditions. Parts of the initial conditions were chosen as in Wynn's epsilon algorithm according to Eq. (3.17). In addition to these epsilon-type initial conditions (3.17), we then needed only one further initial condition for $T_2^{(n)}$, which we identified with Brezinski's theta transformation $\vartheta_2^{(n)}$ according to Eq. (3.18). Thus, our new algorithm (3.20) can be viewed to be essentially a blend of Wynn's epsilon and Brezinski's theta algorithm.

Of course, it should be possible to construct – starting from the generalized recursive scheme (3.12) – alternative new sequence transformations by modifying our choice for $T_2^{(n)}$. The feasibility of this approach will be investigated elsewhere.

Acknowledgements

Y. He was supported by the National Natural Science Foundation of China (Grants no. 11571358), the China Postdoctoral Science Foundation funded project (Grants no. 2012M510186 and 2013T60761), and the Youth Innovation Promotion Association CAS. X.K. Chang was supported by the National Natural Science Foundation of China (Grants no. 11701550, 11731014), and the Youth Innovation Promotion Association CAS. X.B. Hu was supported by the National Natural Science Foundation of China (Grants no. 11371058). J.Q. Sun was supported by the National Natural Science Foundation of China (Grants no. 11401546, 11871444), and the Shandong Provincial Natural Science Foundation, China (Grant no. ZR2013AQ024).

Appendices

A Reduced Bessel functions

In this Appendix, we briefly discuss the most important properties of the so-called reduced Bessel functions [76, Eqs. (3.1) and (3.2)] and their anisotropic generalizations, the so-called *B* functions [42, Eqs. (3.3) and (3.4)]. These functions have gained some prominence in molecular electronic structure theory (see for example [96] and references therein), but have been largely ignored in mathematics. Reduced Bessel and *B* functions had also been the topic of Weniger's Diploma and PhD theses [86, 87]. But in this article, we are predominantly interested in reduced Bessel functions because of the series expansion (A.10) of 1/z in terms of reduced Bessel functions, which is well suited to test the ability of a sequence transformation to accelerate the logarithmic convergence of model sequences of the type of Eq. (2.13) with a non-integral decay parameter.

Based on previous work by Shavitt [71, Eq. (55) on p. 15], the reduced Bessel function with in general complex order v and complex argument z was introduced by Steinborn and Filter [76, Eqs. (3.1) and (3.2)]:

$$\widehat{k}_{\nu}(z) = (2/\pi)^{1/2} z^{\nu} K_{\nu}(z).$$
(A.1)

Here, $K_V(z)$ is a modified Bessel functions of the second kind [59, Eqs. (10.27.4) and (10.27.5)].

Many properties of the reduced Bessel functions follow directly from the corresponding properties of $K_{\rm V}(z)$. One example is the recursion

$$\hat{k}_{\nu+1}(z) = 2\nu \,\hat{k}_{\nu}(z) + z^2 \,\hat{k}_{\nu-1}(z), \tag{A.2}$$

which is stable upwards and which follows directly from the three-term recursion $K_{\nu+1}(z) = (2\nu/z)K_{\nu}(z) + K_{\nu-1}(z)$ [59, Eq. (10.29.1)]. Another example is the symmetry relationship $\hat{k}_{-\nu}(z) = z^{-2\nu}\hat{k}_{\nu}(z)$, which follows from the symmetry relationship $K_{-\nu}(z) = K_{\nu}(z)$ [59, Eq. (10.27.3)].

If the order v of $\hat{k}_v(z)$ is half-integral, v = n + 1/2 with $n \in \mathbb{N}_0$, a reduced Bessel function can be expressed as an exponential multiplied by a terminating confluent hypergeometric series ${}_1F_1$ (see for example [99, Eq. (3.7)]):

$$\widehat{k}_{n+1/2}(z) = 2^n (1/2)_n e^{-z} {}_1F_1(-n; -2n; 2z), \qquad n \in \mathbb{N}_0.$$
 (A.3)

The functions $\hat{k}_{n+1/2}(z)$ can be computed conveniently and reliably with the help of the recursion (A.2) in combination with the starting values $\hat{k}_{-1/2}(z) = e^{-z}/z$ and $\hat{k}_{1/2}(z) = e^{-z}$.

The polynomial part of $\hat{k}_{n+1/2}(z)$ had been considered independently in the mathematical literature. There, the notation

$$\theta_n(z) = e^z \hat{k}_{n+1/2}(z) = 2^n (1/2)_n e^{-z} {}_1F_1(-n; -2n; 2z)$$
(A.4)

is used [48, Eq. (1) on p. 34]. Together with some other, closely related polynomials, the $\theta_n(z)$ are called *Bessel polynomials* [48]. According to Grosswald [48, Section 14], they have been applied in such diverse and seemingly unrelated fields like number theory, statistics, and the analysis of complex electrical networks.

Bessel polynomials occur also in the theory of Padé approximants. Padé [63, p. 82] had shown in his thesis that the Padé approximant $[n/m]_{exp}(z)$ to the exponential function exp(z) can be expressed in closed form, and Baker and Graves-Morris showed that Padé's expression corresponds in modern mathematical notation to the following ratio of two terminating confluent hypergeometric series ${}_{1}F_{1}$ Baker and Graves-Morris [2, Eq. (2.12)]:

$$[n/m]_{\exp}(z) = \frac{{}_{1}F_{1}(-n;-n-m;z)}{{}_{1}F_{1}(-m;-n-m;-z)}, \qquad m,n \in \mathbb{N}_{0}.$$
(A.5)

Thus, the *diagonal* Padé approximants $[n/n]_{exp}(z)$ are ratios of two Bessel polynomials [88, Eq. (14.3-15)]:

$$[n/n]_{\exp}(z) = \frac{\theta_n(z/2)}{\theta_n(-z/2)}, \qquad n \in \mathbb{N}_0.$$
 (A.6)

The known monotonicity properties of the modified Bessel function $K_v(z)$ imply that the reduced Bessel functions $\hat{k}_v(z)$ are for v > 0 and $z \ge 0$ positive and bounded by their values at the origin [99, Eq. (3.1)]. In the case of reduced Bessel functions with half-integral orders, this yields the following bound:

$$0 < k_{n+1/2}(z) \le k_{n+1/2}(0) = 2^n (1/2)_n, \qquad 0 \le z < \infty. \quad n \in \mathbb{N}_0.$$
(A.7)

In Grosswald's book [48], it is shown that for fixed and finite argument z the Bessel polynomials $\theta_n(z)$ satisfy the leading order asymptotic estimate [48, p. 125]

$$\theta_n(z) \sim \frac{(2n)!}{2^n n!} e^z = 2^n (1/2)_n e^z, \qquad n \to \infty.$$
 (A.8)

Combination of Eqs. (A.4) and (A.8) shows that the dominant term of the Poincaré-type asymptotic expansion of $\hat{k}_{n+1/2}(z)$ with fixed and finite argument *z* corresponds to its value at the origin [99, Eq. (3.9)]:

$$\widehat{k}_{n+1/2}(z) = \widehat{k}_{n+1/2}(0) \left[1 + O(n^{-1}) \right] = 2^n (1/2)_n \left[1 + O(n^{-1}) \right], \qquad n \to \infty.$$
(A.9)

For several functions, finite or infinite expansions in terms of reduced Bessel functions are known. As a challenging problem for sequence transformations, we propose to use the series expansion [43, Eq. (6.5)]

$$\frac{1}{z} = \sum_{m=0}^{\infty} \hat{k}_{m-1/2}(z) / [2^m m!], \qquad z > 0.$$
(A.10)

Equation (A.9) implies that the terms $\hat{k}_{m-1/2}(z)/[2^m m!]$ of this series decay like $m^{-3/2}$ as $m \to \infty$ [49, p. 3709], or that the remainders $\sum_{m=n+1}^{\infty} \hat{k}_{m-1/2}(z)/[2^m m!]$ decay like $n^{-1/2}$ as $n \to \infty$. Thus, the series (A.10) converges as slowly as the Dirichlet series $\zeta(s) = \sum_{m=0}^{\infty} (m+1)^s$ with s = 1/2, which is notorious for extremely poor convergence. The slow convergence of the infinite series (A.10) was demonstrated in [49, Table I]. After 10⁶ terms, only 3 decimal digits were correct, which is in agreement with the truncation error estimate given above.

B Levin's transformation

B.1 The general Levin transformation

A sequence transformations of the type of Wynn's epsilon algorithm (2.6) only requires the input of a finite sub-string of a sequence $\{S_n\}_{n=0}^{\infty}$. No additional information is needed for the computation of approximations to the (generalized) limit *S* of an input sequence $\{S_n\}_{n=0}^{\infty}$. Obviously, this is a highly advantageous feature. However, in more fortunate cases, additional information on the index dependence of the truncation errors $R_n = S_n - S$ is available. For example, the truncation errors of Stieltjes series are bounded in magnitude by the first terms neglected in the partial sums (see for example [88, Theorem 13-2]), and they also have the same sign pattern as the first terms neglected. The utilization of such a *structural* information in a transformation process should enhance its efficiency. Unfortunately, there is no obvious way of incorporating such an information into Wynn's recursive epsilon algorithm (2.6) or into other sequence transformations with similar features.

In 1973, Levin [55] introduced a sequence transformation which overcame these limitations and which now bears his name. It uses as input data not only the elements of the sequence $\{S_n\}_{n=0}^{\infty}$, which is to be transformed, but also the elements of another sequence $\{\omega_n\}_{n=0}^{\infty}$ of explicit *estimates* of the remainders $R_n = S_n - S$. These remainders estimates, which must be explicitly known, make it possible to incorporate additional information into the transformation process and are thus ultimately responsible for the remarkable versatility of Levin's transformation.

For Levin's transformation, we use the notation introduced in [88, Eqs. (7.1-6) and (7.1-7)]:

$$\mathscr{L}_{k}^{(n)}(\beta, S_{n}, \omega_{n}) = \frac{\Delta^{k}[(\beta+n)^{k-1}S_{n}/\omega_{n}]}{\Delta^{k}[(\beta+n)^{k-1}/\omega_{n}]}$$
(B.1)
$$\sum_{k=1}^{k} (-1)^{j} \binom{k}{k} \frac{(\beta+n+j)^{k-1}}{2^{k-1}} \frac{S_{n+j}}{2^{k-1}}$$

$$= \frac{\sum_{j=0}^{k} (-1)^{j} \binom{j}{(\beta+n+k)^{k-1}} \overline{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^{j} \binom{k}{j} \frac{(\beta+n+j)^{k-1}}{(\beta+n+k)^{k-1}} \frac{1}{\omega_{n+j}}}, \qquad k,n \in \mathbb{N}_{0}, \quad \beta > 0.$$
(B.2)

Here, $\beta > 0$ is a shift parameter, $\{S_n\}_{n=0}^{\infty}$ is the input sequence, and $\{\omega_n\}_{n=0}^{\infty}$ is a sequence of remainder estimates.

In Eqs. (B.1) and (B.2) it is essential that the input sequence $\{S_n\}$ starts with the sequence element S_0 . The reason is that both the definitions according to Eqs. (B.1) and (B.2) as well as the recurrence formulas for its numerator and denominator sums (see for example[93, Eq. (3.11)]) depend explicitly on *n* as well as on β .

Levin's transformation, which is also discussed in the NIST Handbook [59, §3.9(v) Levin's and Weniger's Transformations], is generally considered to be both a very powerful and a very versatile sequence transformation (see for example [13, 28, 73–75, 88, 93] and references therein). The undeniable success of Levin's transformation inspired others to construct alternative sequence transformations that also use explicit remainder estimates (see for example [36, 52, 88, 90, 93] and references therein).

We still have to discuss the choice of the so far unspecified remainder estimates $\{\omega_n\}_{n=0}^{\infty}$. A principal approach would be to look for remainder estimates that reproduce the leading order asymptotics of the actual remainders [88, Eq. (7.3-1)]:

$$R_n = S_n - S = \omega_n \left[C + O(1/n) \right], \qquad C \neq 0, \quad n \to \infty.$$
(B.3)

This is a completely valid approach, but there is the undeniable problem that for every input sequence $\{S_n\}_{n=0}^{\infty}$ the leading order asymptotics of the corresponding remainders $R_n = S_n - S$ as $n \to \infty$ has to be determined. Unfortunately, such an asymptotic analysis may well lead to some difficult technical problem and be a non-trivial research problem in its own right.

In practice, it is much more convenient to use simple explicit remainder estimates introduced by Levin [55] and Smith and Ford [74], respectively, which are known to work well even in the case of purely numerical input data. In this article, we only consider Levin's remainder estimates $\omega_n = (\beta + n)\Delta S_{n-1}$, and $\omega_n = -[\Delta S_{n-1}][\Delta S_n]/[\Delta^2 S_{n-1}]$, which lead to Levin's *u* and *v* variants [55, Eqs. (58) and (67)]. These estimates lead to transformations that are known to be powerful accelerators for both linear and logarithmic convergence (compare also the asymptotic estimates in [93, Section IV]). Therefore, Levin's *u* and *v* transformations are principally suited to represent the remaining initial condition $T_2^{(n)}$ in Eq. (3.19).

B.2 Levin's *u* transformation

Levin's *u* transformation, which first appeared already in 1936 in the work of Bickley and Miller [10], is characterized by the remainder estimate $\omega_n = (\beta + n)\Delta S_{n-1}$ [55, Eq. (58)]. Inserting this into the finite difference representation (B.1) yields:

$$u_{k}^{(n)}(\beta, S_{n}) = \frac{\Delta^{k}[(\beta+n)^{k-2}S_{n}/\Delta S_{n-1}]}{\Delta^{k}[(\beta+n)^{k-2}/\Delta S_{n-1}]}.$$
(B.4)

For k = 2, the right-hand side of this expression depends on *n* only *implicitly* via the input data $\{S_n\}$ and also does not depend on the scaling parameter β . Thus, we obtain:

$$u_{2}^{(n)}(\beta, S_{n}) = \frac{\Delta^{2}[S_{n}/\Delta S_{n-1}]}{\Delta^{2}[1/\Delta S_{n-1}]}.$$
(B.5)

If we now use $S_n = S_{n-1} + \Delta S_{n-1}$, we obtain $S_n / \Delta S_{n-1} = S_{n-1} / \Delta S_{n-1} + 1$, which implies $\Delta [S_n / \Delta S_{n-1}] = \Delta [S_{n-1} / \Delta S_{n-1}]$. Thus, we obtain the alternative expression,

$$u_2^{(n)}(\beta, S_n) = \frac{\Delta^2[S_{n-1}/\Delta S_{n-1}]}{\Delta^2[1/\Delta S_{n-1}]},$$
(B.6)

which can be reformulated as follows:

$$u_{2}^{(n)}(\beta,S_{n}) = \frac{S_{n}[\Delta S_{n+1}][\Delta^{2}S_{n-1}] - S_{n+1}[\Delta S_{n-1}][\Delta^{2}S_{n}]}{[\Delta S_{n+1}][\Delta^{2}S_{n-1}] - [\Delta S_{n-1}][\Delta^{2}S_{n}]}.$$
(B.7)

In order to enhance numerical stability, it is recommendable to rewrite this expression as follows:

$$u_2^{(n)}(\beta, S_n) = S_n - \frac{\lfloor \Delta S_{n-1} \rfloor \lfloor \Delta S_n \rfloor \lfloor \Delta^2 S_n \rfloor}{\lfloor \Delta S_{n+1} \rfloor \lfloor \Delta^2 S_{n-1} \rfloor - \lfloor \Delta S_{n-1} \rfloor \lfloor \Delta^2 S_n \rfloor}.$$
 (B.8)

B.3 Levin's v transformation

Levin's v transformation is characterized by the remainder estimate [55, Eq. (67)] which is inspired by Aitken's Δ^2 formula (1.8):

$$\omega_n = \frac{[\Delta S_{n-1}][\Delta S_n]}{\Delta S_{n-1} - \Delta S_n} = -\frac{[\Delta S_{n-1}][\Delta S_n]}{\Delta^2 S_{n-1}} = \frac{[\Delta S_{n-1}][\Delta S_n]}{\Delta^2 S_{n-1}}, \quad (B.9)$$

In Eq. (B.9), we made use of the fact that Levin's transformation $\mathscr{L}_{k}^{(n)}(\beta, S_{n}, \omega_{n})$ is a homogeneous function of degree zero of the k + 1 remainder estimates $\omega_{n}, \omega_{n+1}, \ldots$ Thus, we can use any of the expressions in Eq. (B.9) without affecting the value of the transformation.

Inserting the remainder estimate (B.9) into the finite difference representation (B.1) yields:

$$v_{k}^{(n)}(\beta, S_{n}) = \frac{\Delta^{k} \frac{(\beta+n)^{k-1} S_{n}[\Delta^{2} S_{n-1}]}{[\Delta S_{n-1}][\Delta S_{n}]}}{\Delta^{k} \frac{(\beta+n)^{k-1}[\Delta^{2} S_{n-1}]}{[\Delta S_{n-1}][\Delta S_{n}]}}.$$
(B.10)

For k = 1, the right-hand side of this expression depends on *n* only *implicitly* via the input data $\{S_n\}$ and also does not depend on the scaling parameter β . We obtain:

$$v_1^{(n)}(\beta, S_n) = \frac{S_{n+1}[\Delta S_{n-1}][\Delta^2 S_n] - S_n[\Delta S_{n+1}][\Delta^2 S_{n-1}]}{[\Delta S_{n-1}][\Delta^2 S_n] - [\Delta S_{n+1}][\Delta^2 S_{n-1}]}.$$
(B.11)

Comparison of Eqs. (B.7) and (B.11) yields $v_1^{(n)}(\beta, S_n) = u_2^{(n)}(\beta, S_n)$ for arbitrary $\beta \in \mathbb{R}$ and $n \in \mathbb{N}_0$. Again, it is recommendable to rewrite Eq. (B.11) as follows:

$$v_1^{(n)}(\beta, S_n) = S_n + \frac{[\Delta S_n][\Delta S_{n-1}][\Delta^2 S_n]}{[\Delta S_{n-1}][\Delta^2 S_n] - [\Delta S_{n+1}][\Delta^2 S_{n-1}]}.$$
 (B.12)

References

- Aitken AC (1926) On Bernoulli's numerical solution of algebraic equations. Proc Roy Soc Edinburgh 46:289 – 305
- 2. Baker GA Jr, Graves-Morris P (1996) Padé Approximants, 2nd edn. Cambridge U. P., Cambridge
- 3. Barbeau EJ (1979) Euler subdues a very obstreperous series. Amer Math Monthly 86:356 372
- 4. Barbeau EJ, Leah PJ (1976) Euler's 1760 paper on divergent series. Hist Math 3:141 160
- Barber MN, Hamer CJ (1982) Extrapolation of sequences using a generalized epsilon-algorithm. J Austral Math Soc B 23:229 – 240
- 6. Bender CM, Wu TT (1969) Anharmonic oscillator. Phys Rev 184:1231 1260
- 7. Bender CM, Wu TT (1971) Large-order behavior of perturbation theory. Phys Rev Lett 27:461 465
- Bender CM, Wu TT (1973) Anharmonic oscillator. II. A study in perturbation theory in large order. Phys Rev D 7:1620 – 1636
- Bhowmick S, Bhattacharya R, Roy D (1989) Iterations of convergence accelerating nonlinear transforms. Comput Phys Commun 54:31 – 36
- Bickley WG, Miller JCP (1936) The numerical summation of slowly convergent series of positive terms. Phil Mag 22:754 – 767
- 11. Bjørstad P, Dahlquist G, Grosse E (1981) Extrapolations of asymptotic expansions by a modified Aitken δ^2 -formula. BIT 21:56 65
- 12. Borghi R (2016) Computational optics through sequence transformations. In: Visser TD (ed) Progress in Optics, vol 61, Academic Press, Amsterdam, chap 1, pp 1 70
- 13. Borghi R, Weniger EJ (2015) Convergence analysis of the summation of the factorially divergent Euler series by Padé approximants and the delta transformation. Appl Numer Math 94:149 178
- Bornemann F, Laurie D, Wagon S, Waldvogel J (2004) The SIAM 100-Digit Challenge: A Study in High-Accuracy Numerical Computing. Society of Industrial Applied Mathematics, Philadelphia
- Bowman KO, Shenton LR (1989) Continued Fractions in Statistical Applications. Marcel Dekker, New York
- Brezinski C (1971) Accélération de suites à convergence logarithmique. C R Acad Sc Paris 273 A:727 – 730
- 17. Brezinski C (1971) Méthodes d'accélération de la convergence en analyse numérique. Thèse d'Etat, Université de Grenoble
- Brezinski C (1972) Conditions d'application et de convergence de procédés d'extrapolation. Numer Math 20:64 – 79
- 19. Brezinski C (1977) Accélération de la Convergence en Analyse Numérique. Springer-Verlag, Berlin
- Brezinski C (1978) Algorithmes d'Accélération de la Convergence Étude Numérique. Éditions Technip, Paris
- 21. Brezinski C (1980) Padé-Type Approximation and General Orthogonal Polynomials. Birkhäuser, Basel
- 22. Brezinski C (1991) A Bibliography on Continued Fractions, Padé Approximation, Sequence Transformation and Related Subjects. Prensas Universitarias de Zaragoza, Zaragoza
- 23. Brezinski C (1991) History of Continued Fractions and Padé Approximants. Springer-Verlag, Berlin
- Brezinski C (1996) Extrapolation algorithms and Padé approximations: A historical survey. Appl Numer Math 20:299 318
- Brezinski C (2000) Convergence acceleration during the 20th century. J Comput Appl Math 122:1 21. Reprinted in: Brezinski C (ed) Numerical Analysis 2000, Vol. 2: Interpolation and Extrapolation, Elsevier, Amsterdam, pp 1 – 21
- 26. Brezinski C (2009) Some pioneers of extrapolation methods. In: Bultheel A, Cools R (eds) The Birth of Numerical Analysis, World Scientific, Singapore, pp 1 22
- 27. Brezinski C (2019) Reminiscences of Peter Wynn. Numer Algor 80:5 10
- 28. Brezinski C, Redivo Zaglia M (1991) Extrapolation Methods. North-Holland, Amsterdam
- Brezinski C, Redivo Zaglia M (2019) The genesis and early developments of Aitken's process, Shanks transformation, the ε-algorithm, and related fixed point methods. Numer Algor 80:11 – 133
- Brezinski C, Redivo Zaglia M, Weniger EJ (2010) Special Issue: Approximation and extrapolation of convergent and divergent sequences and series (CIRM, Luminy, France, 2009). Appl Numer Math 60:1183 – 1464
- Brezinski C, He Y, Hu XB, Redivo-Zaglia M, Sun JQ (2012) Multistep ε-algorithm, Shanks' transformation, and the Lotka-Volterra system by Hirota's method. Math Comput 81:1527 1549
- Bromwich TJI (1991) An Introduction to the Theory of Infinite Series, 3rd edn. Chelsea, New York, originally published by Macmillan (London, 1908 and 1926).
- Burkhardt H (1911) Über den Gebrauch divergenter Reihen in der Zeit von 1750 1860. Math Annal 70:169 – 206

- Caliceti E, Meyer-Hermann M, Ribeca P, Surzhykov A, Jentschura UD (2007) From useful algorithms for slowly convergent series to physical predictions based on divergent perturbative expansions. Phys Rep 446:1 – 96
- Chang XK, He Y, Hu XB, Li SH (2018) A new integrable convergence acceleration algorithm for computing Brezinski-Durbin-Redivo-Zaglia's sequence transformation via pfaffians. Numer Algor 78:87 – 106
- Čížek J, Zamastil J, Skála L (2003) New summation technique for rapidly divergent perturbation series. Hydrogen atom in magnetic field. J Math Phys 44:962 – 968
- 37. Cuyt A, Wuytack L (1987) Nonlinear Methods in Numerical Analysis. North-Holland, Amsterdam
- 38. Delahaye JP (1988) Sequence Transformations. Springer-Verlag, Berlin
- Drummond JE (1976) Summing a common type of slowly convergent series of positive terms. J Austral Math Soc B 19:416 – 421
- 40. Dyson DJ (1952) Divergence of perturbation theory in quantum electrodynamics. Phys Rev 85:32 33
 41. Ferraro G (2008) The Rise and Development of the Theory of Series up to the Early 1820s. Springer-Verlag, New York
- 42. Filter E, Steinborn EO (1978) Extremely compact formulas for molecular one-electron integrals and Coulomb integrals over Slater-type atomic orbitals. Phys Rev A 18:1 – 11
- Filter E, Steinborn EO (1978) The three-dimensional convolution of reduced Bessel functions and other functions of physical interest. J Math Phys 19:79 – 84
- Fischer J (1997) On the role of power expansions in quantum field theory. Int J Mod Phys A 12:3625 3663
- 45. Gil A, Segura J, Temme NM (2007) Numerical Methods for Special Functions. SIAM, Philadelphia
- 46. Gil A, Segura J, Temme NM (2011) Basic methods for computing special functions. In: Simos TE (ed) Recent Advances in Computational and Applied Mathematics, Springer-Verlag, Dordrecht, pp 67 – 121
- Graves-Morris PR, Roberts DE, Salam A (2000) The epsilon algorithm and related topics. J Comput Appl Math 122:51 – 80. Reprinted in: Brezinski C (ed) Numerical Analysis 2000, Vol. 2: Interpolation and Extrapolation, Elsevier, Amsterdam, pp 51 – 80
- 48. Grosswald E (1978) Bessel Polynomials. Springer-Verlag, Berlin
- Grotendorst J, Weniger EJ, Steinborn EO (1986) Efficient evaluation of infinite-series representations for overlap, two-center nuclear attraction, and Coulomb integrals using nonlinear convergence accelerators. Phys Rev A 33:3706 – 3726
- 50. Hardy GH (1949) Divergent Series. Clarendon Press, Oxford
- He Y, Hu XB, Sun JQ, Weniger EJ (2011) Convergence acceleration algorithm via an equation related to the lattice Boussinesq equation. SIAM J Sci Comput 33:1234 – 1245
- Homeier HHH (2000) Scalar Levin-type sequence transformations. J Comput Appl Math 122:81 147. Reprinted in: Brezinski C (ed) Numerical Analysis 2000, Vol. 2: Interpolation and Extrapolation, Elsevier, Amsterdam, pp 81 – 147
- Kummer EE (1837) Eine neue Methode, die numerischen Summen langsam convergirender Reihen zu berechnen. J Reine Angew Math 16:206 – 214
- 54. Le Guillou JC, Zinn-Justin J (eds) (1990) Large-Order Behaviour of Perturbation Theory. North-Holland, Amsterdam
- Levin D (1973) Development of non-linear transformations for improving convergence of sequences. Int J Comput Math B 3:371 – 388
- 56. Liem CB, Lü T, Shih TM (1995) The Splitting Extrapolation Method. World Scientific, Singapore
- 57. Marchuk GI, Shaidurov VV (1983) Difference Methods and Their Extrapolations. Springer-Verlag, New York
- Nagai A, Satsuma J (1995) Discrete soliton equations and convergence acceleration algorithms. Phys Lett A 209:305 – 312
- Olver FWJ, Lozier DW, Boisvert RF, Clark CW (eds) (2010) NIST Handbook of Mathematical Functions. Cambridge U. P., Cambridge. Available online under http://dlmf.nist.gov/
- Osada N (1990) A convergence acceleration method for some logarithmically convergent sequences. SIAM J Numer Anal 27:178 – 189
- 61. Osada N (1996) An acceleration theorem for the ρ algorithm. Numer Math 73:521 531
- 62. Osada N (2012) The early history of convergence acceleration methods. Numer Algor 60:205 221
- Padé H (1892) Sur la représentation approachée d'une fonction par des fractions rationelles. Ann Sci Éc Norm Sup 9:3 – 93
- Papageorgiou V, Grammaticos B, Ramani A (1993) Integrable lattices and convergence acceleration algorithms. Phys Lett A 179:111 – 115
- Press WH, Teukolsky SA, Vetterling WT, Flannery BP (2007) Numerical Recipes: The Art of Scientific Computing, 3rd edn. Cambridge U. P., Cambridge

- Sablonniere P (1991) Comparison of four algorithms accelerating the convergence of a subset of logarithmic fixed point sequences. Numer Algor 1:177 – 197
- Schmidt JR (1941) On the numerical solution of linear simultaneous equations by an iterative method. Philos Mag 32:369 – 383
- Sedogbo GA (1990) Convergence acceleration of some logarithmic sequences. J Comput Appl Math 32:253 – 260
- Shanks D (1949) An analogy between transient and mathematical sequences and some nonlinear sequence transforms suggested by it. Part I. Tech. rep., Naval Ordonance Laboratory, White Oak, memorandum 9994
- Shanks D (1955) Non-linear transformations of divergent and slowly convergent sequences. J Math and Phys (Cambridge, Mass) 34:1 – 42
- Shavitt I (1963) The Gaussian function in calculations of statistical mechanics and quantum mechanics. In: Alder B, Fernbach S, Rotenberg M (eds) Methods in Computational Physics Vol. 2. Quantum Mechanics, Academic Press, New York, pp 1–45
- 72. Sidi A (2002) A convergence and stability study of the iterated Lubkin transformation and the θ -algorithm. Math Comput 72:419 433
- 73. Sidi A (2003) Practical Extrapolation Methods. Cambridge U. P., Cambridge
- 74. Smith DA, Ford WF (1979) Acceleration of linear and logarithmic convergence. SIAM J Numer Anal 16:223 240
- Smith DA, Ford WF (1982) Numerical comparisons of nonlinear convergence accelerators. Math Comput 38:481 – 499
- 76. Steinborn EO, Filter E (1975) Translations of fields represented by spherical-harmonic expansions for molecular calculations. III. Translations of reduced Bessel functions, Slater-type s-orbitals, and other functions. Theor Chim Acta 38:273 – 281
- 77. Sun JQ, Chang XK, He Y, Hu XB (2013) An extended multistep Shanks transformation and convergence acceleration algorithm with their convergence and stability analysis. Numer Math 125:785 809
- 78. Suslov IM (2005) Divergent perturbation series. J Exp Theor Phys (JETP) 100:1188 1234
- 79. Temme NM (2007) Numerical aspects of special functions. Acta Numer 16:379 478
- Todd J (1962) Motivation for working in numerical analysis. In: Todd J (ed) Survey of Numerical Analysis, McGraw-Hill, New York, pp 1 – 26
- 81. Todd J (1975) The lemniscate constants. Commun ACM 18:14 19
- 82. Trefethen LN (2013) Approximation Theory and Approximation Practice. SIAM, Philadelphia
- Tucciarone J (1973) The development of the theory of summable divergent series from 1880 to 1925. Arch Hist Ex Sci 10:1 – 40
- Vanden Broeck JM, Schwartz LW (1979) A one-parameter family of sequence transformations. SIAM J Math Anal 10:658 – 666
- 85. Walz G (1996) Asymptotics and Extrapolation. Akademie Verlag, Berlin
- 86. Weniger EJ (1977) Untersuchung der Verwendbarkeit reduzierter Besselfunktionen als Basissatz für ab initio Rechnungen an Molekülen. Vergleichende Rechnungen am Beispiel des H₂⁺. Diplomarbeit, Fachbereich Chemie und Pharmazie, Universität Regensburg
- 87. Weniger EJ (1982) Reduzierte Bessel-Funktionen als LCAO-Basissatz: Analytische und numerische Untersuchungen. PhD thesis, Fachbereich Chemie und Pharmazie, Universität Regensburg. A short abstract of this thesis was published in Zentralblatt für Mathematik 523, 444 (1984), abstract no. 65015
- Weniger EJ (1989) Nonlinear sequence transformations for the acceleration of convergence and the summation of divergent series. Comput Phys Rep 10:189 – 371, Los Alamos Preprint math-ph/0306302 (http://arXiv.org)
- Weniger EJ (1991) On the derivation of iterated sequence transformations for the acceleration of convergence and the summation of divergent series. Comput Phys Commun 64:19 – 45
- 90. Weniger EJ (1992) Interpolation between sequence transformations. Numer Algor 3:477 486
- 91. Weniger EJ (1994) Verallgemeinerte Summationsprozesse als numerische Hilfsmittel für quantenmechanische und quantenchemische Rechnungen. Habilitation thesis, Fachbereich Chemie und Pharmazie, Universität Regensburg, Los Alamos Preprint math-ph/0306048 (http://arXiv.org)
- 92. Weniger EJ (2000) Prediction properties of Aitken's iterated Δ^2 process, of Wynn's epsilon algorithm, and of Brezinski's iterated theta algorithm. J Comput Appl Math 122:329 356. Reprinted in: Brezinski C (ed) Numerical Analysis 2000, Vol. 2: Interpolation and Extrapolation, Elsevier, Amsterdam, pp 329 356
- Weniger EJ (2004) Mathematical properties of a new Levin-type sequence transformation introduced by Čížek, Zamastil, and Skála. I. Algebraic theory. J Math Phys 45:1209 – 1246
- 94. Weniger EJ (2007) Further discussion of sequence transformation methods. Subtopic "Related Resources" (R1) on the Numerical Recipes (Third Edition) Webnotes page

http://www.nr.com/webnotes/

- 95. Weniger EJ (2008) On the analyticity of Laguerre series. J Phys A 41:425,207-1-425,207-43
- Weniger EJ (2009) The strange history of *B* functions or how theoretical chemists and mathematicians do (not) interact. Int J Quantum Chem 109:1706 – 1716
- 97. Weniger EJ (2010) An introduction to the topics presented at the conference "Approximation and extrapolation of convergent and divergent sequences and series" CIRM Luminy: September 28, 2009 – October 2, 2009. Appl Numer Math 60:1184 – 1187
- Weniger EJ, Kirtman B (2003) Extrapolation methods for improving the convergence of oligomer calculations to the infinite chain limit of *quasi*-onedimensional stereoregular polymers. Comput Math Applic 45:189 215
- 99. Weniger EJ, Steinborn EO (1983) Numerical properties of the convolution theorems of *B* functions. Phys Rev A 28:2026 2041
- 100. Wimp J (1981) Sequence Transformations and Their Applications. Academic Press, New York
- 101. Wynn P (1956) On a device for computing the $e_m(S_n)$ transformation. Math Tables Aids Comput 10:91 96
- 102. Wynn P (1956) On a Procrustean technique for the numerical transformation of slowly convergent sequences and series. Proc Camb Phil Soc 52:663 671
- 103. Wynn P (1965) A note on programming repeated applications of the ε -algorithm. Rev Franc Trait Inform Chiffres 8:23 62
- 104. Wynn P (1966) On the convergence and the stability of the epsilon algorithm. SIAM J Numer Anal 3:91 - 122