Prediction Properties of Aitken's Iterated Δ^2 Process, of Wynn's Epsilon Algorithm, and of Brezinski's Iterated Theta Algorithm

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Abstract

The prediction properties of Aitken's iterated Δ^2 process, Wynn's epsilon algorithm, and Brezinski's iterated theta algorithm for (formal) power series are analyzed. As a first step, the defining recursive schemes of these transformations are suitably rearranged in order to permit the derivation of accuracy-through-order relationships. On the basis of these relationships, the rational approximants can be rewritten as a partial sum plus an appropriate transformation term. A Taylor expansion of such a transformation term, which is a rational function and which can be computed recursively, produces the predictions for those coefficients of the (formal) power series which were not used for the computation of the corresponding rational approximant.

1 Introduction

In applied mathematics and in theoretical physics, Padé approximants are now used almost routinely to overcome problems with slowly convergent or divergent power series. Of course, there is an extensive literature on Padé approximants: In addition to countless articles, there are several textbooks [5, 6, 8, 17, 28, 41, 44, 52, 73], review articles [3, 4, 9, 24, 25, 55, 119], collections of articles and proceedings [7, 21, 29, 39, 40, 42, 53, 56–58, 78, 112, 114], bibliographies [14, 20, 115], and there is even a book [19] and an article [22], respectively, treating the history of Padé approximants and related topics. A long but by no means complete list of applications of Padé approximants in physics and chemistry can be found in Section 4 of [100].

The revival of the interest in Padé approximants was initiated by two articles by Shanks [84] and Wynn [116], respectively. These articles, which stimulated an enormous amount of research, were published in 1956 at a time when electronic computers started to become more widely available. Shanks [84] introduced a sequence transformation which produces Padé approximants if the input data are the partial sums of a power series, and Wynn [116] showed that this transformation can be computed conveniently and effectively by a recursive scheme now commonly called the epsilon algorithm. As a consequence of the intense research initiated by Shanks [84] and Wynn [116], the mathematical properties of Padé approximants are now fairly well understood, and it is generally accepted that Padé approximants are extremely useful numerical tools which can be applied profitably in a large variety of circumstances.

This intense research of course also showed that Padé approximants have certain limitations and shortcomings. For example, Padé approximants are in principle limited to convergent and divergent power series and cannot help in the case of many other slowly convergent sequences and series with different convergence types.

The convergence type of numerous practically important sequences $\{s_n\}_{n=0}^{\infty}$ can be classified by the asymptotic condition

$$\lim_{n\to\infty} \frac{s_{n+1} - s}{s_n - s} \; = \; \rho \,, \tag{1.1}$$

which closely resembles the well known ratio test for infinite series. Here, $s = s_{\infty}$ is the limit of $\{s_n\}_{n=0}^{\infty}$ as $n \to \infty$. A convergent sequence satisfying (1.1) with $|\rho| < 1$ is called *linearly* convergent, and it is called *logarithmically* convergent if $\rho = 1$. The partial sums of a power series with a nonzero, but finite radius of convergence are a typical example of a linearly convergent sequence. The partial sums of the Dirichlet series for the Riemann zeta function,

$$\zeta(z) \; = \; \sum_{m=0}^{\infty} (m+1)^{-z} \,, \qquad \mathrm{Re}(z) > 1 \,, \tag{1.2}$$

which is notorious for its extremely slow convergence if $\mathrm{Re}(z)$ is only slightly larger than one, are a typical example of a logarithmically convergent sequence.

Padé approximants as well as the closely related epsilon algorithm [116] are known to accelerate effectively the convergence of linearly convergent power series and they are also able to sum many divergent power series. However, they fail completely in the case of logarithmic convergence (compare for example [117, Theorem 12]). Moreover, in the case of divergent power series whose series coefficients grow more strongly than factorially, Padé approximants either converge too slowly to be numerically useful [35, 86] or are not at all able to accomplish a summation to a unique finite generalized limit [54]. Consequently, the articles by Shanks [84] and Wynn [116] also stimulated research on sequence transformations. The rapid progress in this field is convincingly demonstrated by the large number of monographs and review articles on sequence transformations which appeared in recent years [15, 16, 23, 26, 43, 67, 70, 94, 95, 113].

In some, but by no means in all cases, sequence transformations are able to do better than Padé approximants, and it may even happen that they clearly outperform Padé approximants. Thus, it may well be worth while to investigate whether it is possible to use instead

of Padé approximants more specialized sequence transformations which may be better adapted to the problem under consideration. For example, the present author used sequence transformations successfully as computational tools in such diverse fields as the evaluation of special functions [63, 90, 95, 96, 99, 100, 103, 106], the evaluation of molecular multicenter integrals of exponentially decaying functions [59, 61, 100, 109, 111], the summation of strongly divergent quantum mechanical perturbation expansions [33, 34, 36, 96, 98, 100–102, 104–107], and the extrapolation of quantum chemical *ab initio* calculations for oligomers to the infinite chain limit of quasi-onedimensional stereoregular polymers [32, 100, 110]. In vast majority of these applications, it was either not possible to use Padé approximants at all, or alternative sequence transformations did a better job.

In most practical applications of Padé approximants or also of sequence transformations, the partial sums of (formal) power series are transformed into rational approximants with the intention of either accelerating convergence or to accomplish a summation to a finite (generalized) limit in the case of divergence. Padé approximants and sequence transformations are normally not used for the computation of the coefficients of the power series. In the majority of applications, the computation of the coefficients of power series is not the most serious computational problem, and conventional methods for the computation of the coefficients usually suffice.

However, in the case of certain perturbation expansions as they for instance occur in high energy physics, in quantum field theory, or in quantum chromodynamics, the computational problems can be much more severe. Not only do these perturbation expansions, which are power series in some coupling constant, diverge quite strongly for every nonzero value of the coupling constant, but it is also extremely difficult to compute more than just a few of the perturbation series coefficients. Moreover, due to the the complexity of the computations and the necessity of making often drastic approximations, the perturbation series coefficients obtained in this way are usually affected by comparatively large relative errors. Under such adverse circumstances, it has recently become customary to use Padé approximants to make predictions about the leading unknown coefficients of perturbation expansions as well as to make consistency checks for the previously calculated coefficients [27, 30, 31, 46–50, 65, 79–83, 89].

On a heuristic level, the prediction capability of Padé approximants, which was apparently first used by Gilewicz [51], can be explained quite easily. Let us assume that a function f possesses the following (formal) power series,

$$f(z) \; = \; \sum_{\nu=0}^{\infty} \gamma_\nu \, z^\nu \, , \tag{1.3}$$

and that we want to transform the sequence of its partial sums

$$f_n(z) \; = \; \sum_{\nu=0}^{n} \gamma_\nu \, z^\nu \tag{1.4}$$

into a doubly indexed sequence of Padé approximants

$$[l/m]_f(z) \; = \; P_l(z)/Q_m(z) \, . \tag{1.5}$$

As is well known [5, 8], the coefficients of the polynomials $P_l(z) = p_0 + p_1 z + \ldots + p_l z^l$ and $Q_m(z) = 1 + q_1 z + \ldots + q_m z^m$ are chosen in such a way that the Taylor expansion of the Padé approximant agrees as far as possible with the (formal) power series (1.3):

$$f(z) - P_l(z)/Q_m(z) \;=\; O\big(z^{l+m+1}\big)\,, \qquad z \to 0\,. \tag{1.6}$$

This *accuracy-through-order* relationship implies that the Padé approximant to $f(z)$ can be written as the partial sum, from which it was constructed, plus a term which was generated by the transformation of the partial sum to the rational approximant:

$$[l/m]_f(z) \;=\; \sum_{\nu=0}^{l+m} \gamma_\nu \, z^\nu \;+\; z^{l+m+1}\, \mathcal{P}_l^m(z) \;=\; f_{l+m}(z) \;+\; z^{l+m+1}\, \mathcal{P}_l^m(z)\,. \tag{1.7}$$

Similarly, the (formal) power series (1.3) can be expressed as follows:

$$f(z) \;=\; \sum_{\nu=0}^{l+m} \gamma_\nu \, z^\nu \;+\; z^{l+m+1}\, \mathcal{F}_{l+m+1}(z) \;=\; f_{l+m}(z) \;+\; z^{l+m+1}\, \mathcal{F}_{l+m+1}(z)\,. \tag{1.8}$$

Let us now assume that the Padé approximant $[l/m]_f(z)$ provides a sufficiently accurate approximation to $f(z)$. Then, the Padé transformation term $\mathcal{P}_l^m(z)$ must also provide a sufficiently accurate approximation to the truncation error $\mathcal{F}_{l+m+1}(z)$ of the (formal) power series. In general, we have no reason to assume that $\mathcal{P}_l^m(z)$ could be equal to $\mathcal{F}_{l+m+1}(z)$ for finite values of l and m. Consequently, Taylor expansions of $\mathcal{P}_l^m(z)$ and $\mathcal{F}_{l+m+1}(z)$, respectively, will in general produce different results. Nevertheless, the *leading* coefficients of the Taylor expansion for $\mathcal{P}_l^m(z)$ should provide sufficiently accurate approximations to the corresponding coefficients of the Taylor series for $\mathcal{F}_{l+m+1}(z)$.

It is important to note that this prediction capability does not depend on the convergence of the power series expansions for $\mathcal{P}_l^m(z)$ and $\mathcal{F}_{l+m+1}(z)$, respectively. Padé approximants are able to make predictions about series coefficients even if the power series (1.3) for f as well as the power series expansions for $\mathcal{P}_l^m$ and $\mathcal{F}_{l+m+1}(z)$ are only asymptotic as $z \to 0$. This fact explains why the prediction capability of Padé approximants can be so very useful in the case of violently divergent perturbation expansions.

Let us now assume that a sequence transformation also produces a convergent sequence of rational approximants if it acts on the partial sums (1.4) of the (formal) power series (1.3). Then, by the same line of reasoning, these rational approximants should also be able to make predictions about the leading coefficients of the power series, which were not used for the construction of the rational approximant. It seems that these ideas were first formulated by Sidi and Levin [85] and Brezinski [18]. Recently, these ideas were extended by Prévost and Vekemans [72] who discussed prediction methods for sequences which they called ε_p and partial Padé prediction, respectively. Moreover, in [105] it was shown that suitably chosen sequence transformations can indeed make more accurate predictions about unknown power series coefficients than Padé approximants.

Consequently, it should be interesting to analyze the prediction properties of sequence transformations. In this this article, only Aitken's iterated Δ^2 algorithm, Wynn's epsilon algorithm

and the iteration of Brezinski's theta algorithm will be considered. Further studies on the prediction properties of other sequence transformations are in progress and will be presented elsewhere.

If the prediction properties of sequence transformations are to be studied, there is an additional complication which is absent in the case of Padé approximants. The accuracy-through-order relationship (1.6) leads to a system of $l + m + 1$ linear equations for the coefficients of the polynomials $P_l(z) = p_0 + p_1 z + \ldots + p_l z^l$ and $Q_m(z) = 1 + q_1 z + \ldots + q_m z^m$ of the Padé approximant (1.5) [5,8]. If this system of equations has a solution, then it is automatically guaranteed that the Padé approximant obtained in this way satisfies the accuracy-through-order relationship (1.6).

In the case of the sequence transformations considered in this article, the situation is in general more complicated. These transformations are not defined as solutions of systems of linear equations, but via nonlinear recursive schemes. Moreover, their accuracy-through-order relationships are with the exception of Wynn's epsilon algorithm unknown and have to be derived via their defining recursive schemes.

On the basis of these accuracy-through-order relationships, it is possible to construct explicit recursive schemes for the transformation errors as well as for the first coefficient of the power series which was not used for the computation of the rational approximant.

In Section 2, the the accuracy-through-order and prediction properties of Aitken's iterated Δ^2 process are analyzed. In Section 3, the analogous properties of Wynn's epsilon algorithm are discussed, and in Section 4, Brezinski's iterated theta algorithm is treated. In Section 5, some applications of the new results are presented. This article is concluded by Section 6 which contains a short summary.

2 Aitken's Iterated Δ^2 Process

Let us consider the following model sequence:

$$s_n \;=\; s + c\,\lambda^n, \qquad c \neq 0, \quad |\lambda| \neq 1, \quad n \in \mathbb{N}_0. \tag{2.1}$$

For $n \to \infty$, this sequence obviously converges to its limit s if $0 < |\lambda| < 1$, and it diverges away from its generalized limit s if $|\lambda| > 1$.

A sequence transformation, which is able to determine the (generalized) limit s of the model sequence (2.1) from the numerical values of three consecutive sequence elements s_n, s_{n+1} and s_{n+2}, can be constructed quite easily. Just consider s, c, and λ as unknowns of the linear system $s_{n+j} = s + c\lambda^{n+j}$ with $j = 0, 1, 2$. A short calculation shows that

$$\mathcal{A}_1^{(n)} \;=\; s_n - \frac{[\Delta s_n]^2}{\Delta^2 s_n}, \qquad n \in \mathbb{N}_0, \tag{2.2}$$

is able to determine the (generalized) limit of the model sequence (2.1) according to $\mathcal{A}_1^{(n)} = s$. It should be noted that s can be determined in this way, no matter whether the sequence (2.1)

converges or diverges. The forward difference operator Δ in (2.2) is defined by its action on a function $g = g(n)$:

$$\Delta g(n) \;=\; g(n+1) \,-\, g(n)\,. \tag{2.3}$$

The Δ^2 formula (2.2) is certainly one of the oldest sequence transformations. It is usually attributed to Aitken [1], but it is actually much older. Brezinski [19, pp. 90 - 91] mentioned that in 1674 Seki Kowa, the probably most famous Japanese mathematician of that period, tried to obtain better approximations to π with the help of this Δ^2 formula, and according to Todd [91, p. 5] it was in principle already known to Kummer [66].

There is an extensive literature on Aitken's Δ^2 process. For example, it was discussed by Lubkin [68], Shanks [84], Tucker [92, 93], Clark, Gray, and Adams [37], Cordellier [38], Jurkat [64], Bell and Phillips [10], and Weniger [95, Section 5]. A multidimensional generalization of Aitken's transformation to vector sequences was discussed by MacLeod [69]. Modifications and generalizations of Aitken's Δ^2 process were proposed by Drummond [45], Jamieson and O'Beirne [62], Bjørstad, Dahlquist, and Grosse [12], and Sablonniere [76]. Then, there is a close connection between the Aitken process and Fibonacci numbers, as discussed by McCabe and Phillips [71] and Arai, Okamoto, and Kametaka [2]. The properties of Aitken's Δ^2 process are also discussed in books by Baker and Graves-Morris [8], Brezinski [15, 16], Brezinski and Redivo Zaglia [26], Delahaye [43], Walz [94], and Wimp [113].

The power of Aitken's Δ^2 process is of course limited since it is designed to eliminate only a single exponential term. However, its power can be increased considerably by iterating it, yielding the following nonlinear recursive scheme:

$$\mathcal{A}_0^{(n)} \;=\; s_n\,, \qquad n \in \mathbb{N}_0\,, \tag{2.4a}$$

$$\mathcal{A}_{k+1}^{(n)} \;=\; \mathcal{A}_k^{(n)} - \frac{\left[\Delta\mathcal{A}_k^{(n)}\right]^2}{\Delta^2\mathcal{A}_k^{(n)}}\,, \qquad k, n \in \mathbb{N}_0\,. \tag{2.4b}$$

In the case of doubly indexed quantities like $\mathcal{A}_k^{(n)}$, it will always be assumed that the difference operator Δ only acts on the superscript n but not on the subscript k:

$$\Delta\mathcal{A}_k^{(n)} \;=\; \mathcal{A}_k^{(n+1)} \,-\, \mathcal{A}_k^{(n)}\,. \tag{2.5}$$

The numerical performance of Aitken's iterated Δ^2 process was studied in [88, 95]. Concerning the theoretical properties of Aitken's iterated Δ^2 process, very little seems to be known. Hillion [60] was able to find a model sequence for which the iterated Δ^2 process is exact. He also derived a determinantal representation for $\mathcal{A}_k^{(n)}$. However, Hillion's expressions for $\mathcal{A}_k^{(n)}$ contain explicitly the lower order transforms $\mathcal{A}_0^{(n)}, \ldots, \mathcal{A}_{k-1}^{(n)}, \ldots, \mathcal{A}_0^{(n+k)}, \ldots, \mathcal{A}_{k-1}^{(n+k)}$. Consequently, it seems that Hillion's result [60] – although interesting from a formal point of view – cannot help much to analyze the prediction properties of $\mathcal{A}_k^{(n)}$.

If we want to use Aitken's iterated Δ^2 process for the prediction of unknown series coefficients, we first have to derive its accuracy-through-order relationship of the type of (1.6) on the basis of the recursive scheme (2.4).

It is a direct consequence of the recursive scheme (2.4) that $2k + 1$ sequence elements s_n, s_{n+1}, ... , s_{n+2k} are needed for the computation of $\mathcal{A}_k^{(n)}$. Thus, we now choose as input data the partial sums (1.4) of the (formal) power series (1.3) according to $s_n = f_n(z)$, and conjecture that all coefficients γ_0, γ_1, ... , γ_{n+2k}, which were used for the construction of $\mathcal{A}_k^{(n)}$, are exactly reproduced by a Taylor expansion. This means that we have to look for an accuracy-through-order relationship of the following kind:

$$f(z) - \mathcal{A}_k^{(n)} = O\big(z^{n+2k+1}\big), \qquad z \to 0. \tag{2.6}$$

Such an accuracy-through-order relationship would imply that $\mathcal{A}_k^{(n)}$ can be expressed as follows:

$$\mathcal{A}_k^{(n)} = f_{n+2k}(z) + G_k^{(n)} z^{n+2k+1} + O\big(z^{n+2k+2}\big), \qquad z \to 0. \tag{2.7}$$

The constant $G_k^{(n)}$ is the prediction made for the coefficient γ_{n+2k+1}, which is the first coefficient of the power series (1.3) not used for the computation of $\mathcal{A}_k^{(n)}$.

Unfortunately, the recursive scheme (2.4) is not suited for our purposes. This can be shown by computing $\mathcal{A}_1^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, and $f_{n+2}(z)$:

$$\mathcal{A}_1^{(n)} = f_n(z) + \frac{\big[\gamma_{n+1}\big]^2 z^{n+1}}{\gamma_{n+1} - \gamma_{n+2}z}. \tag{2.8}$$

Superficially, it looks as if $\mathcal{A}_1^{(n)}$ is not of the type of (2.7). However, the rational expression on the right-hand side contains the missing terms $\gamma_{n+1}z^{n+1}$ and $\gamma_{n+2}z^{n+2}$. We only have to use $1/(1-y) = 1 + y + y^2/(1-y)$ with $y = \gamma_{n+2}z/\gamma_{n+1}$ to obtain an equivalent expression with the desired features:

$$\mathcal{A}_1^{(n)} = f_{n+2}(z) + \frac{\big[\gamma_{n+2}\big]^2 z^{n+3}}{\gamma_{n+1} - \gamma_{n+2}z}. \tag{2.9}$$

Thus, an expression, which is in agreement with (2.7), can be obtained easily in the case of the simplest transform $\mathcal{A}_1^{(n)}$. Moreover, (2.9) makes the prediction $G_1^{(n)} = \big[\gamma_{n+2}\big]^2/\gamma_{n+1}$ for the first series coefficient γ_{n+3} not used for the computation of $\mathcal{A}_1^{(n)}$. Of course, by expanding the denominator on the right-hand side of (2.9) further predictions on series coefficients with higher indices can be made.

In the case of more complicated transforms $\mathcal{A}_k^{(n)}$ with $k > 1$, it is by no means obvious whether and how the necessary manipulations, which would transform an expression of the type of (2.8) into an expression of the type of (2.9), can be done. Consequently, it is advantageous to replace the recursive scheme (2.4) by an alternative recursive scheme, which directly leads to appropriate expressions for $\mathcal{A}_k^{(n)}$ with $k > 1$.

Many different expressions for $\mathcal{A}_1^{(n)}$ in terms of s_n, s_{n+1}, and s_{n+2} are known [95, Section 5.1]. These expressions are all mathematically equivalent although their numerical properties

may differ. Comparison with (2.9) shows that the for our purposes appropriate expression is [95, Eq. (5.1-7)]

$$\mathcal{A}_1^{(n)} \; = \; s_{n+2} \, - \, \frac{[\Delta s_{n+1}]^2}{\Delta^2 s_n} \, . \tag{2.10}$$

Just like (2.2), this expression can be iterated and yields

$$\mathcal{A}_0^{(n)} \;\; = \;\; s_n \, , \qquad n \in \mathbb{N}_0 \, , \tag{2.11a}$$

$$\mathcal{A}_{k+1}^{(n)} \;\; = \;\; \mathcal{A}_k^{(n+2)} \, - \, \frac{\left[\Delta \mathcal{A}_k^{(n+1)}\right]^2}{\Delta^2 \mathcal{A}_k^{(n)}} \, , \qquad k, n \in \mathbb{N}_0 \, . \tag{2.11b}$$

The recursive schemes (2.4) and (2.11) are mathematically completely equivalent. However, for our purposes – the analysis of the prediction properties of Aitken's iterated Δ^2 process in the case of power series – the recursive scheme (2.11) is much better suited.

Next, we rewrite the partial sums (1.4) of the (formal) power series (1.3) according to

$$f_n(z) \; = \; f(z) \, - \, \sum_{\nu=0}^{\infty} \gamma_{n+\nu+1} \, z^{n+\nu+1} \tag{2.12}$$

and use them as input data in the recursive scheme (2.11). This yields the following expression:

$$\mathcal{A}_k^{(n)} \; = \; f(z) \, + \, z^{n+2k+1} \, R_k^{(n)}(z) \, , \qquad k, n \in \mathbb{N}_0 \, . \tag{2.13}$$

The quantities $R_k^{(n)}(z)$ can be computed with the help of the following recursive scheme which is a direct consequence of the recursive scheme (2.11) for $\mathcal{A}_k^{(n)}$:

$$R_0^{(n)}(z) \;\; = \;\; - \sum_{\nu=0}^{\infty} \gamma_{n+\nu+1} \, z^{\nu} \; = \; \frac{f_n(z) - f(z)}{z^{n+1}} \, , \qquad n \in \mathbb{N}_0 \, , \tag{2.14a}$$

$$R_{k+1}^{(n)}(z) \;\; = \;\; R_k^{(n+2)}(z) \, - \, \frac{\left[\delta R_k^{(n+1)}(z)\right]^2}{\delta^2 R_k^{(n)}(z)} \, , \qquad k, n \in \mathbb{N}_0 \, . \tag{2.14b}$$

In (2.14), we use the shorthand notation

$$\delta X_k^{(n)}(z) \;\; = \;\; z X_k^{(n+1)}(z) \, - \, X_k^{(n)}(z) \, , \tag{2.15a}$$

$$\delta^2 X_k^{(n)}(z) \;\; = \;\; z \delta X_k^{(n+1)}(z) \, - \, \delta X_k^{(n)}(z)$$

$$= \;\; z^2 X_k^{(n+2)}(z) \, - \, 2 z X_k^{(n+1)}(z) \, + \, X_k^{(n)}(z) \, . \tag{2.15b}$$

It seems that we have now accomplished our aim since (2.13) has the right structure to serve as an accuracy-through-order relationship for Aitken's iterated Δ^2 process. Unfortunately, this conclusion is in general premature and we have to require that the input data satisfy some

additional conditions. One must not forget that Aitken's Δ^2 formula (2.10) as well as its iteration (2.11) cannot be applied to arbitrary input data. One obvious potential complication, which has to be excluded, is that (2.11b) becomes undefined if $\Delta^2 \mathcal{A}_k^{(n)} = 0$. Thus, if we want to transform the partial sums (1.4) of the (formal) power series (1.3), it is natural to require that all series coefficients are nonzero, i.e., $\gamma_\nu \neq 0$ for all $\nu \in \mathbb{N}_0$.

Unfortunately, this is only a minimal requirement and not yet enough for our purposes. If $z^{n+2k+1} R_k^{(n)}(z)$ in (2.13) is to be of order $O\big(z^{n+2k+1}\big)$ as $z \to 0$, then the z-independent part $C_k^{(n)}$ of $R_k^{(n)}(z)$ defined by

$$R_k^{(n)}(z) \;=\; C_k^{(n)} + O(z), \qquad z \to 0, \tag{2.16}$$

has to satisfy

$$C_k^{(n)} \;\neq\; 0, \qquad k, n \in \mathbb{N}_0. \tag{2.17}$$

If these conditions are satisfied, we can be sure that (2.13) is indeed the accuracy-through-order relationship we have been looking for.

Personally, I am quite sceptical that it would be easy to characterize *theoretically* those power series which give rise to truncation errors $R_k^{(n)}(z)$ satisfying (2.16) and (2.17). Fortunately, it can easily be checked *numerically* whether a given (formal) power series leads to truncation errors whose z-independent parts are nonzero. If we set $z = 0$ in (2.14) and use (2.16), we obtain the following recursive scheme:

$$C_0^{(n)} \;=\; -\gamma_{n+1}, \qquad n \in \mathbb{N}_0, \tag{2.18a}$$

$$C_{k+1}^{(n)} \;=\; C_k^{(n+2)} - \frac{\big[C_k^{(n+1)}\big]^2}{C_k^{(n)}}, \qquad k, n \in \mathbb{N}_0. \tag{2.18b}$$

Let us now assume that we know for a given (formal) power series that the z-independent parts $C_k^{(n)}$ of the truncation errors $R_k^{(n)}(z)$ in (2.13) are nonzero – either from a mathematical proof or from a brute force calculation using (2.18). Then, (2.13) is indeed the accuracy-through-order relationship we have been looking for, which implies that $\mathcal{A}_k^{(n)}$ can be expressed as follows:

$$\mathcal{A}_k^{(n)} \;=\; f_{n+2k}(z) + z^{n+2k+1}\, \Phi_k^{(n)}(z), \qquad k, n \in \mathbb{N}_0. \tag{2.19}$$

If we use this ansatz in (2.11), we obtain the following recursive scheme:

$$\Phi_0^{(n)}(z) \;=\; 0, \qquad n \in \mathbb{N}_0, \tag{2.20a}$$

$$\Phi_{k+1}^{(n)}(z) \;=\; \Phi_k^{(n+2)}(z) - \frac{\big[\gamma_{n+2k+2} + \delta\Phi_k^{(n+1)}(z)\big]^2}{\gamma_{n+2k+2}z - \gamma_{n+2k+1} + \delta^2\Phi_k^{(n)}(z)}, \qquad k, n \in \mathbb{N}_0. \tag{2.20b}$$

Here, $\delta\Phi_k^{(n)}(z)$ and $\delta^2\Phi_k^{(n)}(z)$ are defined by (2.15). For $k = 0$, (2.20b) yields

$$\Phi_1^{(n)}(z) \;=\; \frac{\big[\gamma_{n+2}\big]^2}{\gamma_{n+1} - \gamma_{n+2}z}, \tag{2.21}$$

which is in agreement with (2.9).

A comparison of (2.7) and (2.19) yields

$$\Phi_k^{(n)}(z) \; = \; G_k^{(n)} + O(z)\,, \qquad z \to 0\,. \tag{2.22}$$

Consequently, the z-independent part $G_k^{(n)}$ of $\Phi_k^{(n)}(z)$ is the prediction for the first coefficient γ_{n+2k+1} not used for the computation of $\mathcal{A}_k^{(n)}$.

If we set $z = 0$ in the recursive scheme (2.20) and use (2.22), we obtain the following recursive scheme for the predictions $G_k^{(n)}$:

$$\begin{align}
G_0^{(n)} &= 0\,, \qquad n \in \mathbb{N}_0\,, \tag{2.23a} \\
G_1^{(n)} &= \left[\gamma_{n+2}\right]^2 / \gamma_{n+1}\,, \qquad n \in \mathbb{N}_0\,, \tag{2.23b} \\
G_{k+1}^{(n)} &= G_k^{(n+2)} + \frac{\left[\gamma_{n+2k+2} - G_k^{(n+1)}\right]^2}{\gamma_{n+2k+1} - G_k^{(n)}}\,, \qquad k, n \in \mathbb{N}_0\,. \tag{2.23c}
\end{align}$$

The z-independent parts $C_k^{(n)}$ of $R_k^{(n)}(z)$ and $G_k^{(n)}$ of $\Phi_k^{(n)}(z)$, respectively, are connected. A comparison of (2.13), (2.16), (2.19), and (2.22) yields:

$$G_k^{(n)} \; = \; C_k^{(n)} + \gamma_{n+2k+1}\,. \tag{2.24}$$

In this article, rational approximants will always be used in such a way that the input data – the partial sums (1.4) of the (formal) power series (1.3) – are computed in an outer loop, and for each new partial sum a new approximation to the limit is calculated. If the index m of the last partial sum $f_m(z)$ is even, $m = 2\mu$, we use in the case of Aitken's iterated Δ^2 process as approximation to the limit $f(z)$ the transformation

$$\left\{ f_0(z), f_1(z), \dots, f_{2\mu}(z) \right\} \mapsto \mathcal{A}_\mu^{(0)}\,, \tag{2.25}$$

and if m is odd, $m = 2\mu + 1$, we use the transformation

$$\left\{ f_1(z), f_2(z), \dots, f_{2\mu+1}(z) \right\} \mapsto \mathcal{A}_\mu^{(1)}\,. \tag{2.26}$$

With the help of the notation $[\![x]\!]$ for the integral part of x, which is the largest integer ν satisfying the inequality $\nu \le x$, these two relationships can be combined into a single equation, yielding [95, Eq. (5.2-6)]

$$\left\{ f_{m-2[\![m/2]\!]}(z), f_{m-2[\![m/2]\!]+1}(z), \dots, f_m(z) \right\} \mapsto \mathcal{A}_{[\![m/2]\!]}^{(m-2[\![m/2]\!])}\,, \qquad m \in \mathbb{N}_0\,. \tag{2.27}$$

The same strategy will also be used if for example the rational expressions $R_k^{(n)}(z)$ defined by (2.13) are listed in a Table. This means that the $R_k^{(n)}(z)$ will also be listed according to (2.27). The only difference is that the $R_k^{(n)}(z)$ use as input data not the partial sums $f_n(z)$ but the remainders $[f_n(z) - f(z)]/z^{n+1}$.

3 Wynn's Epsilon Algorithm

Wynn's epsilon algorithm [116] is the following nonlinear recursive scheme:

$$\epsilon_{-1}^{(n)} = 0, \qquad \epsilon_0^{(n)} = s_n, \qquad n \in \mathbb{N}_0, \tag{3.1a}$$

$$\epsilon_{k+1}^{(n)} = \epsilon_{k-1}^{(n+1)} + 1/[\epsilon_k^{(n+1)} - \epsilon_k^{(n)}], \qquad k, n \in \mathbb{N}_0. \tag{3.1b}$$

The elements $\epsilon_{2k}^{(n)}$ with *even* subscripts provide approximations to the (generalized) limit s of the sequence $\{s_n\}_{n=0}^\infty$ to be transformed, whereas the elements $\epsilon_{2k+1}^{(n)}$ with *odd* subscripts are only auxiliary quantities which diverge if the whole process converges.

If the input data are the partial sums (1.4) of the (formal) power series (1.3), $s_n = f_n(z)$, then Wynn [116] could show that his epsilon algorithm produces Padé approximants:

$$\epsilon_{2k}^{(n)} = [n + k/k]_f(z). \tag{3.2}$$

The epsilon algorithm is a close relative of Aitken's iterated Δ^2 process, and they have similar properties in convergence acceleration and summation processes. A straightforward calculation shows that $\mathcal{A}_1^{(n)} = \epsilon_2^{(n)}$. Hence, Aitken's iterated Δ^2 process may also be viewed as an iteration of $\epsilon_2^{(n)}$. However, for $k > 1$, $\mathcal{A}_k^{(n)}$ and $\epsilon_{2k}^{(n)}$ are in general different.

There is an extensive literature on the epsilon algorithm. On p. 120 of Wimps book [113] it is mentioned that over 50 articles on the epsilon algorithm were published by Wynn alone, and at least 30 articles by Brezinski. As a fairly complete source of references Wimp recommends Brezinski's first book [15]. However, this book was published in 1977, and since then many more articles on the epsilon algorithm have been published. Consequently, any attempt to produce something resembling a reasonably complete bibliography of Wynn's epsilon algorithm would clearly be beyond the scope of this article.

In spite of its numerous advantageous features, Wynn's epsilon algorithm (3.1) is not suited for our purposes. If the input data are the partial sums (1.4) of the (formal) power series (1.3), the accuracy-through-order relationship (1.6) of Padé approximants in combination with (3.2) implies that the elements of the epsilon table with even subscripts can be expressed as

$$\epsilon_{2k}^{(n)} = f_{n+2k}(z) + g_{2k}^{(n)} z^{n+2k+1} + O(z^{n+2k+2}), \qquad z \to 0. \tag{3.3}$$

The constant $g_{2k}^{(n)}$ is the prediction made for the coefficient γ_{n+2k+1}, which is the first coefficient of the power series (1.3) not used for the computation of $\epsilon_{2k}^{(n)}$.

If we compute $\epsilon_2^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, and $f_{n+2}(z)$, we obtain because of $\mathcal{A}_1^{(n)} = \epsilon_2^{(n)}$ the same expressions as in the last section. Thus, we obtain a result which does not seem to be in agreement with the accuracy-through-order relationship (3.3):

$$\epsilon_2^{(n)} = f_{n+1}(z) + \frac{\gamma_{n+1}\gamma_{n+2}z^{n+2}}{\gamma_{n+1} - \gamma_{n+2}z}. \tag{3.4}$$

Of course, the missing term $\gamma_{n+2}z^{n+2}$ can easily be extracted from the rational expression on the right-hand side. We only have to use $1/(1-y) = 1 + y/(1-y)$ with $y = \gamma_{n+2}z/\gamma_{n+1}$ to obtain as in the case of Aitken's iterated Δ^2 algorithm an expression with the desired features:

$$\epsilon_2^{(n)} \;=\; f_{n+2}(z) \;+\; \frac{\left[\gamma_{n+2}\right]^2 z^{n+3}}{\gamma_{n+1} - \gamma_{n+2}z}\,. \tag{3.5}$$

This example shows that the accuracy-through-order relationship (1.6) of Padé approximants is by no means immediately obvious from the epsilon algorithm (3.1). A further complication is that the epsilon algorithm involves the elements $\epsilon_{2k+1}^{(n)}$ with odd subscripts. These are only auxiliary quantities which diverge if the whole process converges. Nevertheless, they make it difficult to obtain order estimates and to reformulate the epsilon algorithm in such a way that it automatically produces suitable expressions for $\epsilon_{2k}^{(n)}$ of the type of (3.5).

The starting point for the construction of an alternative recursive scheme, which would be suited for our purposes, is Wynn's cross rule [118, Eq. (13)]:

$$\left\{\epsilon_{2k+2}^{(n)} - \epsilon_{2k}^{(n+1)}\right\}^{-1} \;+\; \left\{\epsilon_{2k-2}^{(n+2)} - \epsilon_{2k}^{(n+1)}\right\}^{-1}$$

$$=\; \left\{\epsilon_{2k}^{(n)} - \epsilon_{2k}^{(n+1)}\right\}^{-1} \;+\; \left\{\epsilon_{2k}^{(n+2)} - \epsilon_{2k}^{(n+1)}\right\}^{-1}\,. \tag{3.6}$$

This expression permits the recursive computation of the elements $\epsilon_{2k}^{(n)}$ with even subscripts without having to compute the auxiliary quantities $\epsilon_{2k+1}^{(n)}$ with odd subscripts. The price, one has to pay, is that the cross rule (3.6) has a more complicated structure than the extremely simple epsilon algorithm (3.1).

A further complication is that for $k = 0$ the undefined element $\epsilon_{-2}^{(n)}$ occurs in (3.6). However, we obtain results that are consistent with Wynn's epsilon algorithm (3.1) if we set $\epsilon_{-2}^{(n)} = \infty$.

Hence, instead of the epsilon algorithm (3.1), we can also use the following recursive scheme:

$$\epsilon_{-2}^{(n)} \;=\; \infty\,, \qquad \epsilon_0^{(n)} \;=\; s_n\,, \qquad n \in \mathbb{N}_0\,, \tag{3.7a}$$

$$\epsilon_{2k+2}^{(n)} \;=\; \epsilon_{2k}^{(n+1)} \;+\; \cfrac{1}{\cfrac{1}{\Delta\epsilon_{2k}^{(n+1)}} - \cfrac{1}{\Delta\epsilon_{2k}^{(n)}} + \cfrac{1}{\epsilon_{2k}^{(n+1)} - \epsilon_{2k-2}^{(n+2)}}}\,, \qquad k, n \in \mathbb{N}_0\,. \tag{3.7b}$$

For our purposes, this recursive scheme is an improvement over the epsilon algorithm (3.1) since it does not contain the elements $\epsilon_{2k+1}^{(n)}$ with odd subscripts. Nevertheless, it is not yet what we need. The use of (3.7) for the computation of $\epsilon_2^{(n)}$ would produce (3.4) but not (3.5). Fortunately, (3.7) can easily be modified to yield a recursive scheme having the desired features:

$$\epsilon_{-2}^{(n)} = \infty, \qquad \epsilon_0^{(n)} = s_n, \qquad n \in \mathbb{N}_0, \tag{3.8a}$$

$$\epsilon_{2k+2}^{(n)} = \epsilon_{2k}^{(n+2)} + \frac{\dfrac{\Delta\epsilon_{2k}^{(n+1)}}{\Delta\epsilon_{2k}^{(n)}} - \dfrac{\Delta\epsilon_{2k}^{(n+1)}}{\epsilon_{2k}^{(n+1)} - \epsilon_{2k-2}^{(n+2)}}}{\dfrac{1}{\Delta\epsilon_{2k}^{(n+1)}} - \dfrac{1}{\Delta\epsilon_{2k}^{(n)}} + \dfrac{1}{\epsilon_{2k}^{(n+1)} - \epsilon_{2k-2}^{(n+2)}}}, \qquad k, n \in \mathbb{N}_0. \tag{3.8b}$$

If we use (3.8) for the computation of $\epsilon_2^{(n)}$, we obtain (3.5).

Next, we use in (3.8) the partial sums (1.4) of the (formal) power series (1.3) in the form of (2.12). This yields:

$$\epsilon_{2k}^{(n)} = f(z) + z^{n+2k+1} r_{2k}^{(n)}(z), \qquad k, n \in \mathbb{N}_0. \tag{3.9}$$

The quantities $r_{2k}^{(n)}(z)$ can be computed with the help of the following recursive scheme which is a direct consequence of the recursive scheme (3.8) for $\epsilon_{2k}^{(n)}$:

$$r_0^{(n)}(z) = -\sum_{\nu=0}^{\infty} \gamma_{n+\nu+1}\, z^{\nu} = \frac{f_n(z) - f(z)}{z^{n+1}}, \qquad n \in \mathbb{N}_0, \tag{3.10a}$$

$$r_2^{(n)}(z) = r_0^{(n+2)}(z) + \frac{\dfrac{\delta r_0^{(n+1)}(z)}{\delta r_0^{(n)}(z)}}{\dfrac{1}{\delta r_0^{(n+1)}(z)} - \dfrac{z}{\delta r_0^{(n)}(z)}}, \qquad n \in \mathbb{N}_0, \tag{3.10b}$$

$$r_{2k+2}^{(n)}(z) = r_{2k}^{(n+2)}(z) + \frac{\dfrac{\delta r_{2k}^{(n+1)}(z)}{\delta r_{2k}^{(n)}(z)} - \dfrac{\delta r_{2k}^{(n+1)}(z)}{z r_{2k}^{(n+1)}(z) - r_{2k-2}^{(n+2)}(z)}}{\dfrac{1}{\delta r_{2k}^{(n+1)}(z)} - \dfrac{z}{\delta r_{2k}^{(n)}(z)} + \dfrac{z}{z r_{2k}^{(n+1)}(z) - r_{2k-2}^{(n+2)}(z)}}, \quad k, n \in \mathbb{N}_0. \tag{3.10c}$$

Here, $\delta r_{2k}^{(n)}(z)$ is defined by (2.15). It should be noted that (3.10b) follows from (3.10c) if we define $r_{-2}^{(n)}(z) = \infty$.

Similar to the analogous accuracy-through-order relationship (2.13) for Aitken's iterated Δ^2 process, (3.9) has the right structure to serve as an accuracy-through-order relationship for Wynn's epsilon algorithm. Thus, it seems that we have accomplished our aim. However, we are faced with the same complications as in the case of (2.13). If $z^{n+2k+1} r_{2k}^{(n)}(z)$ in (3.9) is to be of order $O(z^{n+2k+1})$ as $z \to 0$, then the z-independent part $c_{2k}^{(n)}$ of $r_{2k}^{(n)}(z)$ defined by

$$r_{2k}^{(n)}(z) = c_{2k}^{(n)} + O(z), \qquad z \to 0, \tag{3.11}$$

has to satisfy

$$c_{2k}^{(n)} \neq 0, \qquad k, n \in \mathbb{N}_0. \tag{3.12}$$

If this condition is satisfied, we can be sure that (3.9) is indeed the accuracy-through-order relationship we have been looking for.

As in the case of Aitken's iterated Δ^2 process, it is by no means obvious whether and how it can be proven that a given power series gives rise to truncation errors $r_{2k}^{(n)}(z)$ satisfying (3.11) and (3.12). Fortunately, it can easily be checked *numerically* whether a given (formal) power series leads to truncations errors whose z-independent parts are nonzero. If we set $z = 0$ in (3.10) and use (3.11), we obtain the following recursive scheme:

$$c_0^{(n)} = -\gamma_{n+1}, \qquad n \in \mathbb{N}_0, \tag{3.13a}$$

$$c_2^{(n)} = c_0^{(n+2)} - \frac{\left[c_0^{(n+1)}\right]^2}{c_0^{(n)}}, \qquad n \in \mathbb{N}_0, \tag{3.13b}$$

$$c_{2k+2}^{(n)} = c_{2k}^{(n+2)} - \frac{\left[c_{2k}^{(n+1)}\right]^2}{c_{2k}^{(n)}} + \frac{\left[c_{2k}^{(n+1)}\right]^2}{c_{2k-2}^{(n+2)}}, \qquad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{3.13c}$$

If we define $c_{-2}^{(n)} = \infty$, then (3.13b) follows from (3.13c).

Let us now assume that we know for a given (formal) power series that the z-independent parts $c_{2k}^{(n)}$ of the truncation errors $r_{2k}^{(n)}(z)$ in (3.9) are nonzero – either from a mathematical proof or from a brute force calculation using (3.13). Then, (3.9) is indeed the accuracy-through-order relationship we have been looking for. This implies that $\epsilon_{2k}^{(n)}$ can be expressed as follows:

$$\epsilon_{2k}^{(n)} = f_{n+2k}(z) + z^{n+2k+1} \varphi_{2k}^{(n)}(z). \tag{3.14}$$

If we use this ansatz in (3.8), we obtain the following recursive scheme:

$$\varphi_0^{(n)}(z) = 0, \qquad n \in \mathbb{N}_0, \tag{3.15a}$$

$$\varphi_2^{(n)}(z) = \frac{\left[\gamma_{n+2}\right]^2}{\gamma_{n+1} - \gamma_{n+2}z}, \qquad n \in \mathbb{N}_0, \tag{3.15b}$$

$$\varphi_{2k+2}^{(n)}(z) = \varphi_{2k}^{(n+2)}(z) + \frac{\alpha_{2k+2}^{(n)}(z)}{\beta_{2k+2}^{(n)}(z)}, \qquad k \in \mathbb{N}, \quad n \in \mathbb{N}_0, \tag{3.15c}$$

$$\alpha_{2k+2}^{(n)}(z) = \frac{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)}{\gamma_{n+2k+1} + \delta\varphi_{2k}^{(n)}(z)} - \frac{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)}{\gamma_{n+2k+1} + z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k-2}^{(n+2)}(z)}, \tag{3.15d}$$

$$\beta_{2k+2}^{(n)}(z) = \frac{1}{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)} - \frac{z}{\gamma_{n+2k+1} + \delta\varphi_{2k}^{(n)}(z)}$$
$$+ \frac{z}{\gamma_{n+2k+1} + z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k-2}^{(n+2)}(z)}. \tag{3.15e}$$

Here, $\delta\varphi_{2k}^{(n)}(z)$ is defined by (2.15). Moreover, we could also define $\varphi_{-2}^{(n)}(z) = \infty$. Then, (3.15b) would follow from (3.15c).

A comparison of (3.3) and (3.14) yields

$$\varphi_{2k}^{(n)}(z) \;=\; g_{2k}^{(n)} \,+\, O(z)\,, \qquad z \to 0\,. \tag{3.16}$$

Consequently, the z-independent part $g_{2k}^{(n)}$ of $\varphi_{2k}^{(n)}(z)$ is the prediction for the first coefficient γ_{n+2k+1} not used for the computation of $\epsilon_{2k}^{(n)}$.

If we set $z = 0$ in the recursive scheme (3.15) and use (3.16), we obtain the following recursive scheme for the predictions $g_{2k}^{(n)}$:

$$g_0^{(n)} \;=\; 0\,, \qquad n \in \mathbb{N}_0\,, \tag{3.17a}$$

$$g_2^{(n)} \;=\; \frac{\big[\gamma_{n+2}\big]^2}{\gamma_{n+1}}\,, \qquad n \in \mathbb{N}_0\,, \tag{3.17b}$$

$$g_{2k+2}^{(n)} \;=\; g_{2k}^{(n+2)} \,+\, \frac{\big[\gamma_{n+2k+2} - g_{2k}^{(n+1)}\big]^2}{\gamma_{n+2k+1} - g_{2k}^{(n)}} \,-\, \frac{\big[\gamma_{n+2k+2} - g_{2k}^{(n+1)}\big]^2}{\gamma_{n+2k+1} - g_{2k-2}^{(n+2)}}\,,$$
$$k \in \mathbb{N}\,, \qquad n \in \mathbb{N}_0\,. \tag{3.17c}$$

If we define $g_{-2}^{(n)} = \infty$, then (3.17b) follows from (3.17a) and (3.17c).

The z-independent parts $c_{2k}^{(n)}$ of $r_{2k}^{(n)}(z)$ and $g_{2k}^{(n)}$ of $\varphi_{2k}^{(n)}(z)$, respectively, are connected. A comparison of (3.9), (3.11), (3.14), and (3.16) yields:

$$g_{2k}^{(n)} \;=\; c_{2k}^{(n)} \,+\, \gamma_{n+2k+1}\,. \tag{3.18}$$

Concerning the choice of the approximation to the limit, we proceed in the case of the epsilon algorithm just like in the case of Aitken's iterated Δ^2 process and compute a new approximation to the limit after the computation of each new partial sum. Thus, if the index m of the last partial sum $f_m(z)$ is even, $m = 2\mu$, we use as approximation to the limit $f(z)$ the transformation

$$\big\{f_0(z), f_1(z), \dots, f_{2\mu}(z)\big\} \mapsto \epsilon_{2\mu}^{(0)}\,, \tag{3.19}$$

and if m is odd, $m = 2\mu + 1$, we use the transformation

$$\big\{f_1(z), f_2(z), \dots, f_{2\mu+1}(z)\big\} \mapsto \epsilon_{2\mu}^{(1)}\,. \tag{3.20}$$

These two relationships can be combined into a single equation, yielding [95, Eq. (4.3-6)]

$$\big\{f_{m-2[\![m/2]\!]}(z), f_{m-2[\![m/2]\!]+1}(z), \dots, f_m(z)\big\} \mapsto \epsilon_{2[\![m/2]\!]}^{(m-2[\![m/2]\!])}\,, \qquad m \in \mathbb{N}_0\,. \tag{3.21}$$

4   The Iteration of Brezinski's Theta Algorithm

Brezinski's theta algorithm is the following recursive scheme [13]:

$$\vartheta_{-1}^{(n)} \;=\; 0\,, \qquad \vartheta_0^{(n)} \;=\; s_n\,, \qquad n \in \mathbb{N}_0\,, \tag{4.1a}$$

$$\vartheta_{2k+1}^{(n)} \;=\; \vartheta_{2k-1}^{(n+1)} + 1/\big[\Delta\vartheta_{2k}^{(n)}\big]\,, \qquad k, n \in \mathbb{N}_0\,, \tag{4.1b}$$

$$\vartheta_{2k+2}^{(n)} \;=\; \vartheta_{2k}^{(n+1)} + \frac{\big[\Delta\vartheta_{2k}^{(n+1)}\big]\big[\Delta\vartheta_{2k+1}^{(n+1)}\big]}{\Delta^2\vartheta_{2k+1}^{(n)}}\,, \qquad k, n \in \mathbb{N}_0\,. \tag{4.1c}$$

As in the case of Wynn's epsilon algorithm (3.1), only the elements $\vartheta_{2k}^{(n)}$ with even subscripts provide approximations to the (generalized) limit of the sequence to be transformed. The elements $\vartheta_{2k+1}^{(n)}$ with odd subscripts are only auxiliary quantities which diverge if the whole process converges.

The theta algorithm was derived from Wynn's epsilon algorithm (3.1) with the intention of overcoming the inability of the epsilon algorithm to accelerate logarithmic convergence. In that respect, the theta algorithm was a great success. Extensive numerical studies of Smith and Ford [87, 88] showed that the theta algorithm is not only very powerful, but also much more versatile than the epsilon algorithm. Like the epsilon algorithm, it is an efficient accelerator for linear convergence and it is also able to sum many divergent series. However, it is also able to accelerate the convergence of many logarithmically convergent sequences and series.

As for example discussed in [97], new sequence transformations can be constructed by iterating explicit expressions for sequence transformations with low transformation orders. The best known example of such an iterated sequence transformation is probably Aitken's iterated Δ^2 process (2.4) which is obtained by iterating Aitken's Δ^2 formula (2.2).

The same approach is also possible in the case of the theta algorithm. A suitable closed-form expression, which may be iterated, is [95, Eq. (10.3-1)]

$$\vartheta_2^{(n)} \;=\; s_{n+1} - \frac{\big[\Delta s_n\big]\big[\Delta s_{n+1}\big]\big[\Delta^2 s_{n+1}\big]}{\big[\Delta s_{n+2}\big]\big[\Delta^2 s_n\big] - \big[\Delta s_n\big]\big[\Delta^2 s_{n+1}\big]}\,, \qquad n \in \mathbb{N}_0\,. \tag{4.2}$$

The iteration of this expression yields the following nonlinear recursive scheme [95, Eq. (10.3-6)]:

$$\mathcal{J}_0^{(n)} \;=\; s_n\,, \qquad n \in \mathbb{N}_0\,, \tag{4.3a}$$

$$\mathcal{J}_{k+1}^{(n)} \;=\; \mathcal{J}_k^{(n+1)} - \frac{\big[\Delta\mathcal{J}_k^{(n)}\big]\big[\Delta\mathcal{J}_k^{(n+1)}\big]\big[\Delta^2\mathcal{J}_k^{(n+1)}\big]}{\big[\Delta\mathcal{J}_k^{(n+2)}\big]\big[\Delta^2\mathcal{J}_k^{(n)}\big] - \big[\Delta\mathcal{J}_k^{(n)}\big]\big[\Delta^2\mathcal{J}_k^{(n+1)}\big]}\,, \qquad k, n \in \mathbb{N}_0\,. \tag{4.3b}$$

In convergence acceleration and summation processes, the iterated transformation $\mathcal{J}_k^{(n)}$ has similar properties as the theta algorithm from which it was derived: They are both very powerful as well as very versatile. $\mathcal{J}_k^{(n)}$ is not only an effective accelerator for linear convergence as

well as able to sum divergent series, but it is also able to accelerate the convergence of many logarithmically convergent sequences and series [11, 74–77, 95, 97, 100].

In spite of all these similarities, the iterated transformation $\mathcal{J}_k^{(n)}$ has one undeniable advantage over the theta algorithm, which ultimately explains why in this article only $\mathcal{J}_k^{(n)}$ is studied, but not the theta algorithm: The recursive scheme (4.3) for $\mathcal{J}_k^{(n)}$ is slightly less complicated than the recursive scheme (4.1) for the theta algorithm. On p. 282 of [95] it was emphasized that a replacement of (4.1b) by the simpler recursion

$$\vartheta_{2k+1}^{(n)} \;=\; 1/\big[\Delta\vartheta_{2k}^{(n)}\big]\,, \qquad k,n \in \mathbb{N}_0\,, \tag{4.4}$$

would lead to a modified theta algorithm which satisfies $\vartheta_{2k}^{(n)} = \mathcal{J}_k^{(n)}$.

It is a direct consequence of the recursive scheme (4.3) that $3k + 1$ sequence elements s_n, s_{n+1}, ... , s_{n+3k} are needed for the computation of $\mathcal{J}_k^{(n)}$. Thus, we now choose as input data the partial sums (1.4) of the (formal) power series (1.3) according to $s_n = f_n(z)$, and conjecture that all coefficients γ_0, γ_1, ... , γ_{n+3k}, which were used for the construction of $\mathcal{J}_k^{(n)}$, are exactly reproduced by a Taylor expansion. This means that we have to look for an accuracy-through-order relationship of the following kind:

$$f(z) \;-\; \mathcal{J}_k^{(n)} \;=\; O\big(z^{n+3k+1}\big)\,, \qquad z \to 0\,. \tag{4.5}$$

Such an accuracy-through-order relationship would imply that $\mathcal{J}_k^{(n)}$ can be expressed as follows:

$$\mathcal{J}_k^{(n)} \;=\; f_{n+3k}(z) \;+\; \mathcal{G}_k^{(n)}\, z^{n+3k+1} \;+\; O\big(z^{n+3k+2}\big)\,, \qquad z \to 0\,. \tag{4.6}$$

The constant $\mathcal{G}_k^{(n)}$ is the prediction made for the coefficient γ_{n+3k+1}, which is the first coefficient of the power series (1.3) not used for the computation of $\mathcal{J}_k^{(n)}$.

Unfortunately, the recursive scheme (4.3) is not suited for our purposes. This can be shown by computing $\mathcal{J}_1^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, $f_{n+2}(z)$, and $f_{n+3}(z)$:

$$\mathcal{J}_1^{(n)} \;=\; f_{n+1}(z) \;-\; \frac{\gamma_{n+1}\gamma_{n+2}\big[\gamma_{n+3}z - \gamma_{n+2}\big]z^{n+2}}{\gamma_{n+3}z\big[\gamma_{n+2}z - \gamma_{n+1}\big] - \gamma_{n+1}\big[\gamma_{n+3}z - \gamma_{n+2}\big]}\,. \tag{4.7}$$

Superficially, it looks as if the accuracy-through-order relationship (4.5) is not satisfied by $\mathcal{J}_1^{(n)}$. However, the rational expression on the right-hand side contains the missing terms $\gamma_{n+2}z^{n+2}$ and $\gamma_{n+3}z^{n+3}$, as shown by the Taylor expansion

$$-\frac{\gamma_{n+1}\gamma_{n+2}\big[\gamma_{n+3}z - \gamma_{n+2}\big]z^{n+2}}{\gamma_{n+3}z\big[\gamma_{n+2}z - \gamma_{n+1}\big] - \gamma_{n+1}\big[\gamma_{n+3}z - \gamma_{n+2}\big]}$$

$$=\; \gamma_{n+2}z^{n+2} \;+\; \gamma_{n+3}z^{n+3} \;-\; \frac{\gamma_{n+3}\Big\{\big[\gamma_{n+2}\big]^2 - 2\gamma_{n+1}\gamma_{n+3}\Big\}z^{n+4}}{\gamma_{n+1}\gamma_{n+2}} \;+\; O\big(z^{n+5}\big)\,. \tag{4.8}$$

Thus, an expression, which is in agreement with (4.6), can be obtained easily in the case of the simplest transform $\mathcal{J}_1^{(n)}$. Moreover, the Taylor expansion (4.8) shows that $\mathcal{J}_1^{(n)}$ makes the prediction

$$\mathcal{G}_1^{(n)} = -\frac{\gamma_{n+3}\left\{\left[\gamma_{n+2}\right]^2 - 2\gamma_{n+1}\gamma_{n+3}\right\}}{\gamma_{n+1}\gamma_{n+2}} \tag{4.9}$$

for the first series coefficient γ_{n+4} not used for the computation of $\mathcal{J}_1^{(n)}$. Of course, by including additional terms in the Taylor expansion (4.8) further predictions on series coefficients with higher indices can be made.

However, in the case of more complicated transforms $\mathcal{J}_k^{(n)}$ with $k > 1$ it by no means obvious whether and how an expression, which is in agreement with (4.6), can be constructed. Consequently, it is certainly a good idea to replace the recursive scheme (4.3) by an alternative recursive scheme, which directly leads to appropriate expressions for $\mathcal{J}_k^{(n)}$ with $k > 1$.

Many different expressions for $\vartheta_2^{(n)}$ in terms of s_n, s_{n+1}, s_{n+2}, and s_{n+3} are known [95, Section 10.4]. The for our purposes appropriate expression is

$$\vartheta_2^{(n)} = s_{n+3} - \frac{\left[\Delta s_{n+2}\right]\left\{\left[\Delta s_{n+2}\right]\left[\Delta^2 s_n\right] + \left[\Delta s_{n+1}\right]^2 - \left[\Delta s_{n+2}\right]\left[\Delta s_n\right]\right\}}{\left[\Delta s_{n+2}\right]\left[\Delta^2 s_n\right] - \left[\Delta s_n\right]\left[\Delta^2 s_{n+1}\right]}. \tag{4.10}$$

Just like (4.2), this expression can be iterated and yields

$$\mathcal{J}_0^{(n)} = s_n, \qquad n \in \mathbb{N}_0, \tag{4.11a}$$

$$\mathcal{J}_{k+1}^{(n)} = \mathcal{J}_k^{(n+3)} - \frac{A_{k+1}^{(n)}}{B_{k+1}^{(n)}}, \qquad k, n \in \mathbb{N}_0, \tag{4.11b}$$

$$A_{k+1}^{(n)} = \left[\Delta \mathcal{J}_k^{(n+2)}\right]\left\{\left[\Delta \mathcal{J}_k^{(n+2)}\right]\left[\Delta^2 \mathcal{J}_k^{(n)}\right] + \left[\Delta \mathcal{J}_k^{(n+1)}\right]^2 \right.$$
$$\left. - \left[\Delta \mathcal{J}_k^{(n)}\right]\left[\Delta \mathcal{J}_k^{(n+2)}\right]\right\}, \tag{4.11c}$$

$$B_{k+1}^{(n)} = \left[\Delta \mathcal{J}_k^{(n+2)}\right]\left[\Delta^2 \mathcal{J}_k^{(n)}\right] - \left[\Delta \mathcal{J}_k^{(n)}\right]\left[\Delta^2 \mathcal{J}_k^{(n+1)}\right]. \tag{4.11d}$$

If we now use either (4.10) or (4.11) to compute $\mathcal{J}_1^{(n)}$ from the partial sums $f_n(z)$, $f_{n+1}(z)$, $f_{n+2}(z)$, and $f_{n+3}(z)$, we obtain the following expression which obviously possesses the desired features:

$$\mathcal{J}_1^{(n)} = f_{n+3}(z) - \frac{\gamma_{n+3}\left\{\gamma_{n+3}\left[\gamma_{n+2}z - \gamma_{n+1}\right] + \left[\gamma_{n+2}\right]^2 - \gamma_{n+1}\gamma_{n+3}\right\}z^{n+4}}{\gamma_{n+3}z\left[\gamma_{n+2}z - \gamma_{n+1}\right] - \gamma_{n+1}\left[\gamma_{n+3}z - \gamma_{n+2}\right]}. \tag{4.12}$$

Next, we use in (4.11) the partial sums (1.4) of the (formal) power series (1.3) in the form of (2.12). This yields:

$$\mathcal{J}_k^{(n)} = f(z) + z^{n+3k+1}\mathcal{R}_k^{(n)}(z), \qquad k, n \in \mathbb{N}_0. \tag{4.13}$$

The quantities $\mathcal{R}_k^{(n)}(z)$ can be computed with the help of the following recursive scheme which is a direct consequence of the recursive scheme (4.11) for $\mathcal{J}_k^{(n)}$:

$$\mathcal{R}_0^{(n)}(z) = -\sum_{\nu=0}^{\infty} \gamma_{n+\nu+1} z^{\nu} = \frac{f_n(z) - f(z)}{z^{n+1}}, \qquad n \in \mathbb{N}_0, \tag{4.14a}$$

$$\mathcal{R}_{k+1}^{(n)}(z) = \mathcal{R}_k^{(n+3)}(z) - \frac{\mathcal{N}_{k+1}^{(n)}(z)}{\mathcal{D}_{k+1}^{(n)}(z)}, \qquad k, n \in \mathbb{N}_0, \tag{4.14b}$$

$$\mathcal{N}_{k+1}^{(n)}(z) = \left[\delta\mathcal{R}_k^{(n+2)}(z)\right]\left\{\left[\delta\mathcal{R}_k^{(n+2)}(z)\right]\left[\delta^2\mathcal{R}_k^{(n)}(z)\right] + \left[\delta\mathcal{R}_k^{(n+1)}(z)\right]^2 \right.$$
$$\left. - \left[\delta\mathcal{R}_k^{(n)}(z)\right]\left[\delta\mathcal{R}_k^{(n+2)}(z)\right]\right\}, \tag{4.14c}$$

$$\mathcal{D}_{k+1}^{(n)}(z) = z\left[\delta\mathcal{R}_k^{(n+2)}(z)\right]\left[\delta^2\mathcal{R}_k^{(n)}(z)\right] - \left[\delta\mathcal{R}_k^{(n)}(z)\right]\left[\delta^2\mathcal{R}_k^{(n+1)}(z)\right]. \tag{4.14d}$$

Here, $\delta\mathcal{R}_k^{(n+2)}(z)$ and $\delta^2\mathcal{R}_k^{(n+2)}(z)$ are defined by (2.15).

Similar to the analogous accuracy-through-order relationships (2.13) and (3.9) for Aitken's iterated Δ^2 process and the epsilon algorithm, respectively, (4.13) has the right structure to serve as an accuracy-through-order relationship for the iterated theta algorithm. Thus, it seems that we have accomplished our aim. However, we are faced with the same complications as in the case of (2.13) and (3.9). If $z^{n+3k+1}\mathcal{R}_{2k}^{(n)}(z)$ in (4.13) is to be of order $O(z^{n+3k+1})$ as $z \to 0$, then the z-independent part $\mathcal{C}_k^{(n)}$ of $\mathcal{R}_k^{(n)}(z)$ defined by

$$\mathcal{R}_k^{(n)}(z) = \mathcal{C}_k^{(n)} + O(z), \qquad z \to 0, \tag{4.15}$$

has to satisfy

$$\mathcal{C}_k^{(n)} \neq 0, \qquad k, n \in \mathbb{N}_0. \tag{4.16}$$

If this condition is satisfied, then it is guaranteed that (4.13) is indeed the accuracy-through-order relationship we have been looking for.

As in the case of Aitken's iterated Δ^2 process or the epsilon algorithm, it is by no means obvious whether and how it can be proven that a given power series gives rise to truncation errors $\mathcal{R}_k^{(n)}(z)$ satisfying (4.15) and (4.16). Fortunately, it can easily be checked *numerically* whether a given (formal) power series leads to truncations errors whose z-independent parts are nonzero. If we set $z = 0$ in (4.14) and use (4.15), we obtain the following recursive scheme:

$$\mathcal{C}_0^{(n)} = -\gamma_{n+1}, \qquad n \in \mathbb{N}_0, \tag{4.17a}$$

$$\mathcal{C}_{k+1}^{(n)} = \mathcal{C}_k^{(n+3)} - \frac{\mathcal{C}_k^{(n+2)}\left\{2\mathcal{C}_k^{(n)}\mathcal{C}_k^{(n+2)} - \left[\mathcal{C}_k^{(n+1)}\right]^2\right\}}{\mathcal{C}_k^{(n)}\mathcal{C}_k^{(n+1)}}, \qquad k, n \in \mathbb{N}_0. \tag{4.17b}$$

Let us now assume that we know for a given (formal) power series that the z-independent parts $\mathcal{G}_k^{(n)}$ of the truncation errors $\mathcal{R}_k^{(n)}(z)$ in (4.13) are nonzero – either from a mathematical

proof or from a brute force calculation using (4.17). Then, (4.13) is indeed the accuracy-through-order relationship we have been looking for. This implies that $\mathcal{J}_k^{(n)}$ can be expressed as follows:

$$\mathcal{J}_k^{(n)} \;=\; f_{n+3k}(z) \,+\, z^{n+3k+1}\,\Psi_k^{(n)}(z)\,, \qquad k,n \in \mathbb{N}_0\,. \tag{4.18}$$

If we use this ansatz in (4.11), we obtain the following recursive scheme:

$$\Psi_0^{(n)}(z) \;=\; 0\,, \qquad n \in \mathbb{N}_0\,, \tag{4.19a}$$

$$\Psi_1^{(n)}(z) \;=\; -\,\frac{\gamma_{n+3}\Big\{\gamma_{n+3}\big[\gamma_{n+2}z - \gamma_{n+1}\big] + \big[\gamma_{n+2}\big]^2 - \gamma_{n+1}\gamma_{n+3}\Big\}}{\gamma_{n+3}\big[\gamma_{n+2}z - \gamma_{n+1}\big] - \gamma_{n+1}\big[\gamma_{n+3}z - \gamma_{n+2}\big]}\,, \qquad n \in \mathbb{N}_0\,, \tag{4.19b}$$

$$\Psi_{k+1}^{(n)}(z) \;=\; \Psi_k^{(n+3)}(z) \,-\, \frac{N_{k+1}^{(n)}(z)}{D_{k+1}^{(n)}(z)}\,, \qquad k,n \in \mathbb{N}_0\,, \tag{4.19c}$$

$$\begin{aligned}
N_{k+1}^{(n)}(z) \;=\;& \big[\gamma_{n+3k+3} + \delta\Psi_k^{(n+2)}(z)\big] \\
&\times \Big\{ \big[\gamma_{n+3k+3} + \delta\Psi_k^{(n+2)}(z)\big]\big[\gamma_{n+3k+2}z - \gamma_{n+3k+1} + \delta^2\Psi_k^{(n)}(z)\big] \\
&\qquad + \big[\gamma_{n+3k+2} + \delta\Psi_k^{(n+1)}(z)\big]^2 \\
&\qquad\quad - \big[\gamma_{n+3k+1} + \delta\Psi_k^{(n)}(z)\big]\big[\gamma_{n+3k+3} + \delta\Psi_k^{(n+2)}(z)\big] \Big\}\,, \tag{4.19d}
\end{aligned}$$

$$\begin{aligned}
D_{k+1}^{(n)}(z) \;=\;& \big[\gamma_{n+3k+3} + \delta\Psi_k^{(n+2)}(z)\big]\big[\gamma_{n+3k+2}z - \gamma_{n+3k+1} + \delta^2\Psi_k^{(n)}(z)\big] \\
&- \big[\gamma_{n+3k+1} + \delta\Psi_k^{(n)}(z)\big]\big[\gamma_{n+3k+3}z - \gamma_{n+3k+2} + \delta^2\Psi_k^{(n+1)}(z)\big]\,. \tag{4.19e}
\end{aligned}$$

Here, $\delta\Psi_k^{(n+2)}(z)$ and $\delta^2\Psi_k^{(n+2)}(z)$ are defined by (2.15).

A comparison of (4.6) and (4.18) yields

$$\Psi_k^{(n)}(z) \;=\; \mathcal{G}_k^{(n)} \,+\, O(z)\,, \qquad z \to 0\,. \tag{4.20}$$

Consequently, the z-independent part $\mathcal{G}_k^{(n)}$ of $\Psi_k^{(n)}(z)$ is the prediction for the first coefficient γ_{n+3k+1} not used for the computation of $\mathcal{J}_k^{(n)}$.

If we set $z = 0$ in the recursive scheme (4.19) and use (4.20), we obtain the following recursive

scheme for the predictions $\mathcal{G}_k^{(n)}$:

$$\mathcal{G}_0^{(n)} = 0, \qquad n \in \mathbb{N}_0, \tag{4.21a}$$

$$\mathcal{G}_1^{(n)} = -\frac{\gamma_{n+3}\left\{\left[\gamma_{n+2}\right]^2 - 2\gamma_{n+1}\gamma_{n+3}\right\}}{\gamma_{n+1}\gamma_{n+2}}, \qquad n \in \mathbb{N}_0, \tag{4.21b}$$

$$\mathcal{G}_{k+1}^{(n)} = \mathcal{G}_k^{(n+3)} - \frac{F_{k+1}^{(n)}}{H_{k+1}^{(n)}}, \qquad k, n \in \mathbb{N}_0, \tag{4.21c}$$

$$F_{k+1}^{(n)} = \left[\gamma_{n+3k+3} - \mathcal{G}_k^{(n+2)}\right]\left\{\left[\gamma_{n+3k+2} - \mathcal{G}_k^{(n+1)}\right]^2\right.$$
$$\left. - 2\left[\gamma_{n+3k+1} - \mathcal{G}_k^{(n)}\right]\left[\gamma_{n+3k+3} - \mathcal{G}_k^{(n+2)}\right]\right\}, \tag{4.21d}$$

$$H_{k+1}^{(n)} = \left[\gamma_{n+3k+1} - \mathcal{G}_k^{(n)}\right]\left[\gamma_{n+3k+2} - \mathcal{G}_k^{(n+1)}\right]. \tag{4.21e}$$

The z-independent parts $\mathcal{C}_k^{(n)}$ of $\mathcal{R}_k^{(n)}(z)$ and $\mathcal{G}_k^{(n)}$ of $\Psi_k^{(n)}(z)$, respectively, are connected. A comparison of (4.13), (4.15), (4.18), and (4.20) yields:

$$\mathcal{G}_k^{(n)} = \mathcal{C}_k^{(n)} + \gamma_{n+3k+1}. \tag{4.22}$$

As in the case of Aitken's iterated Δ^2 process or Wynn's epsilon algorithm, a new approximation to the limit will be computed after the computation of each new partial sum. Thus, if the index m of the last partial sum $f_m(z)$ is a multiple of 3, $m = 3\mu$, we use as approximation to the limit $f(z)$ the transformation

$$\left\{f_0(z), f_1(z), \dots, f_{3\mu}(z)\right\} \mapsto J_\mu^{(0)}, \tag{4.23}$$

if we have $m = 3\mu + 1$, we use the transformation

$$\left\{f_1(z), f_2(z), \dots, f_{3\mu+1}(z)\right\} \mapsto \mathcal{J}_\mu^{(1)}, \tag{4.24}$$

and if we have $m = 3\mu + 2$, we use the transformation

$$\left\{f_2(z), f_3(z), \dots, f_{3\mu+2}(z)\right\} \mapsto \mathcal{J}_\mu^{(2)}, \tag{4.25}$$

These three relationships can be combined into a single equation, yielding [95, Eq. (10.4-7)]

$$\left\{f_{m-3[\![m/3]\!]}(z), f_{m-3[\![m/3]\!]+1}(z), \dots, f_m(z)\right\} \mapsto \mathcal{J}_{[\![m/3]\!]}^{(m-3[\![m/3]\!])}, \qquad m \in \mathbb{N}_0. \tag{4.26}$$

5 Applications

In this article, two principally different kinds of results were derived. The first group of results – the accuracy-through-order relationships (2.13), (3.9), and (4.13) and the corresponding recursive schemes (2.14), (3.9), and (4.14) – defines the transformation error terms $z^{n+2k+1}R_k^{(n)}(z)$,

$z^{n+2k+1}r_{2k}^{(n)}(z)$, and $z^{n+3k+1}\mathcal{R}_k^{(n)}(z)$. These quantities describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\epsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the function $f(z)$ which is to be approximated. Obviously, the transformation error terms must vanish if the transformation process converges.

The second group of results – (2.19), (3.14), and (4.18) and the corresponding recursive schemes (2.20), (3.15), and (4.19) – defines the terms $z^{n+2k+1}\Phi_k^{(n)}(z)$, $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$, and $z^{n+3k+1}\Psi_k^{(n)}(z)$. These quantities describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\epsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the partial sums $f_{n+2k}(z)$ and $f_{n+3k}(z)$, respectively, from which they were constructed. Hence, the first group of results essentially describes what is still missing in the transformation process, whereas the second group describes what was gained by constructing rational expressions from the partial sums.

The recursive schemes (2.14), (3.9), and (4.14) of the first group use as input data the remainder terms

$$\frac{f_n(z) - f(z)}{z^{n+1}} = -\sum_{\nu=0}^{\infty} \gamma_{n+\nu+1} z^\nu. \tag{5.1}$$

In most practically relevant convergence acceleration and summation problems, only a finite number of series coefficients γ_ν are known. Consequently, the remainder terms (5.1) are usually not known explicitly, which means that the immediate practical usefulness of the first group of results is quite limited. Nevertheless, these results are of interest because they can be used to study the convergence of the sequence transformations of this article for model problems.

As an example, let us consider the following series expansion for the logarithm,

$$\frac{\ln(1+z)}{z} = {}_2F_1(1,1;2;-z) = \sum_{m=0}^{\infty} \frac{(-z)^m}{m+1}, \tag{5.2}$$

which converges for all $z \in \mathbb{C}$ with $|z| < 1$. The logarithm possesses the integral representation

$$\frac{\ln(1+z)}{z} = \int_0^1 \frac{dt}{1+zt}, \tag{5.3}$$

which shows that $\ln(1+z)/z$ is a Stieltjes function and that the hypergeometric series on the right-hand side of (5.2) is the corresponding Stieltjes series (a detailed treatment of Stieltjes functions and Stieltjes series can for example be found in Section 5 of [8]). Consequently, $\ln(1+z)/z$ possesses the following representation as a partial sum plus an explicit remainder which is given by a Stieltjes integral (compare for example Eq. (13.1-5) of [95]):

$$\frac{\ln(1+z)}{z} = \sum_{\nu=0}^{n} \frac{(-z)^m}{m+1} + (-z)^{n+1} \int_0^1 \frac{t^{n+1}dt}{1+zt}, \qquad n \in \mathbb{N}_0. \tag{5.4}$$

For $|z| < 1$, the numerator of the remainder integral on the right-hand side can be expanded. Interchanging summation and integration then yields:

$$(-1)^{n+1} \int_0^1 \frac{t^{n+1}dt}{1+zt} = \sum_{m=0}^{\infty} \frac{(-1)^{n+m+1}z^m}{n+m+2}. \tag{5.5}$$

Next, we use for $0 \leq n \leq 6$ the negative of these remainder integrals as input data in the recursive schemes (2.14), (3.9), and (4.14), and do a Taylor expansion of the resulting expressions. Thus, we obtain according to (2.13), (3.9), and (4.13):

$$\mathcal{A}_3^{(0)} = \frac{\ln(1+z)}{z} + \frac{421z^7}{16537500} - \frac{796321z^8}{8682187500} + \frac{810757427z^9}{4051687500000} + O\big(z^{10}\big), \quad \text{(5.6a)}$$

$$\epsilon_6^{(0)} = \frac{\ln(1+z)}{z} + \frac{z^7}{9800} - \frac{31z^8}{77175} + \frac{113z^9}{120050} + O\big(z^{10}\big), \quad \text{(5.6b)}$$

$$\mathcal{J}_2^{(0)} = \frac{\ln(1+z)}{z} + \frac{z^7}{37800} - \frac{19z^8}{198450} + \frac{z^9}{4725} + O\big(z^{10}\big). \quad \text{(5.6c)}$$

All calculations were done symbolically, using the exact rational arithmetics of Maple. Consequently, the results in (5.6) are exact and free of rounding errors.

The leading coefficients of the Taylor expansions of the transformation error terms for $\mathcal{A}_3^{(0)}$ and $\mathcal{J}_2^{(0)}$ are evidently smaller than the corresponding coefficients for $\epsilon_6^{(0)}$. This observation provides considerable evidence that Aitken's iterated Δ^2 process and Brezinski's iterated theta algorithm are in the case of the series (5.2) for $\ln(1+z)/z$ more effective than Wynn's epsilon algorithm which according to (3.2) produces Padé approximants.

This conclusion is also confirmed by the following numerical example in Table I, in which the convergence of the series (5.2) for $\ln(1+z)/z$ is accelerated for $z = 0.95$. The numerical values of the remainder terms (5.5) were used as input data in the recursive schemes (2.14), (3.9), and (4.14) to compute numerically the transformation error terms in (2.13), (3.9), and (4.13). The transformation error terms, which are listed in columns 3 - 5, were chosen in agreement with (2.27), (3.21), and (4.26), respectively.

The zeros, which are found in columns 3 - 5 of Table I, occur because Aitken's iterated Δ^2 process and Wynn's epsilon algorithm can only compute a rational approximant if at least three consecutive partial sums are available, and because the iteration of Brezinski's theta algorithm requires at least four partial sums.

The result in Table I show once more that Aitken's iterated Δ^2 process and Brezinski's iterated theta algorithm are in the case of the series (5.2) for $\ln(1+z)/z$ apparently more effective than Wynn's epsilon algorithm.

The second group of results of this article – (2.19), (3.14), and (4.18) and the corresponding recursive schemes (2.20), (3.15), and (4.19) – can for example be used to demonstrate how rational approximants work if a divergent power series is to be summed.

Let us therefore assume that the partial sums, which occur in (2.19), (3.14), and (4.18), diverge if the index becomes large. Then, a summation to a finite generalized limit $f(z)$ can only be accomplished if $z^{n+2k+1}\Phi_k^{(n)}(z)$ and $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$ in (2.19) and (3.14), respectively, converge to the negative of $f_{n+2k}(z)$, and if $z^{n+3k+1}\Psi_k^{(n)}(z)$ in (4.18) converges to the negative of $f_{n+3k}(z)$.

Table II shows that this is indeed the case. We again consider the infinite series (5.2) for $\ln(1+z)/z$, but this time we choose $z = 5.0$, which is clearly outside the circle of convergence. We use the numerical values of the partial sums $\sum_{m=0}^{n}(-z)^m/(m+1)$ with $0 \leq n \leq 10$ as input

Table I: Convergence of the Transformation Error Terms
Transformation of $\ln(1+z)/z = \sum_{m=0}^{\infty}(-z)^m/(m+1)$ for $z=0.95$

n	$\sum_{m=0}^{\infty}\frac{(-1)^{n+m}z^m}{n+m+2}$	$z^{n+1}R_{[\![n/2]\!]}^{(n-2[\![n/2]\!])}(z)$	$z^{n+1}r_{2[\![n/2]\!]}^{(n-2[\![n/2]\!])}(z)$	$z^{n+1}\mathcal{R}_{[\![n/3]\!]}^{(n-3[\![n/3]\!])}(z)$
		Eq. (2.13)	Eq. (3.9)	Eq. (4.13)
0	$0.312654 \cdot 10^0$	0	0	0
1	$-0.197206 \cdot 10^0$	0	0	0
2	$0.143292 \cdot 10^0$	$0.620539 \cdot 10^{-2}$	$0.620539 \cdot 10^{-2}$	0
3	$-0.112324 \cdot 10^0$	$-0.230919 \cdot 10^{-2}$	$-0.230919 \cdot 10^{-2}$	$0.113587 \cdot 10^{-2}$
4	$0.922904 \cdot 10^{-1}$	$0.109322 \cdot 10^{-3}$	$0.156975 \cdot 10^{-3}$	$-0.367230 \cdot 10^{-3}$
5	$-0.782908 \cdot 10^{-1}$	$-0.333267 \cdot 10^{-4}$	$-0.466090 \cdot 10^{-4}$	$0.148577 \cdot 10^{-3}$
6	$0.679646 \cdot 10^{-1}$	$0.131240 \cdot 10^{-5}$	$0.413753 \cdot 10^{-5}$	$0.137543 \cdot 10^{-5}$
7	$-0.600373 \cdot 10^{-1}$	$-0.371684 \cdot 10^{-6}$	$-0.108095 \cdot 10^{-5}$	$-0.392983 \cdot 10^{-6}$
8	$0.537619 \cdot 10^{-1}$	$0.111500 \cdot 10^{-7}$	$0.110743 \cdot 10^{-6}$	$0.131377 \cdot 10^{-6}$
9	$-0.486717 \cdot 10^{-1}$	$-0.311899 \cdot 10^{-8}$	$-0.266535 \cdot 10^{-7}$	$0.412451 \cdot 10^{-9}$
10	$0.444604 \cdot 10^{-1}$	$0.689220 \cdot 10^{-10}$	$0.298638 \cdot 10^{-8}$	$-0.139178 \cdot 10^{-9}$
11	$-0.409189 \cdot 10^{-1}$	$-0.199134 \cdot 10^{-10}$	$-0.678908 \cdot 10^{-9}$	$0.475476 \cdot 10^{-10}$
12	$0.378992 \cdot 10^{-1}$	$0.282138 \cdot 10^{-12}$	$0.808737 \cdot 10^{-10}$	$-0.316716 \cdot 10^{-12}$

data in the recursive schemes (2.20), (3.15), and (4.19) to compute the transformation terms in (2.19), (3.14), and (4.18). The transformation terms, which are listed in columns 3 - 5 of Table II, were chosen in agreement with (2.27), (3.21), and (4.26), respectively. All calculations were done using the floating point arithmetics of Maple.

The results in Table II show that a sequence transformation accomplishes a summation of a divergent series by constructing approximations to the actual remainders. Both the partial sums as well as the actual remainders diverge individually if their indices become large, but the linear combination of the partial sum and the remainder has a constant and finite value for every index.

The fact, that the transformation terms in (2.19), (3.14), and (4.18) approach the negative of the corresponding partial sums of course also implies that one should not try to sum a divergent series in this way. The subtraction of two nearly equal terms would inevitably lead to a serious loss of significant digits.

In the next example, the transformation terms in (2.19), (3.14), and (4.18) will be used to make predictions for unknown series coefficients. For that purpose, it is recommendable to use a computer algebra system like Maple, and do all calculations symbolically. If the coefficients of the series to be transformed are exact rational numbers, the resulting rational expressions are then computed exactly.

We use the symbolic expressions for the partial sums $\sum_{m=0}^{n}(-z)^m/(m+1)$ with $0 \le n \le 12$ of the infinite series (5.2) for $\ln(1+z)/z$ as input data in the recursive schemes (2.20), (3.15), and (4.19). The resulting rational expressions $z^{13}\Phi_6^{(0)}(z)$, $z^{13}\varphi_{12}^{(0)}(z)$, and $z^{13}\Psi_4^{(4)}$ with unspecified

Table II: Convergence of Transformation Terms to the Partial Sums
Transformation of $\ln(1+z)/z = \sum_{m=0}^{\infty}(-z)^m/(m+1)$ for $z = 5.0$

n	$\sum_{m=0}^{n} \frac{(-z)^m}{m+1}$	$z^{n+1}\Phi_{[\![n/2]\!]}^{(n-2[\![n/2]\!])}(z)$ Eq. (2.19)	$z^{n+1}\varphi_{2[\![n/2]\!]}^{(n-2[\![n/2]\!])}(z)$ Eq. (3.14)	$z^{n+1}\Psi_{[\![n/3]\!]}^{(n-3[\![n/3]\!])}(z)$ Eq. (4.18)
0	$0.1000000000 \cdot 10^1$	0	0	0
1	$-0.1500000000 \cdot 10^1$	0	0	0
2	$0.6833333333 \cdot 10^1$	$-0.6410256410 \cdot 10^1$	$-0.6410256410 \cdot 10^1$	0
3	$-0.2441666667 \cdot 10^2$	$0.2467105263 \cdot 10^2$	$0.2467105263 \cdot 10^2$	$0.2480158730 \cdot 10^2$
4	$0.1005833333 \cdot 10^3$	$-0.1002174398 \cdot 10^3$	$-0.1002155172 \cdot 10^3$	$-0.1002604167 \cdot 10^3$
5	$-0.4202500000 \cdot 10^3$	$0.4205996885 \cdot 10^3$	$0.4205974843 \cdot 10^3$	$0.4206730769 \cdot 10^3$
6	$0.1811892857 \cdot 10^4$	$-0.1811533788 \cdot 10^4$	$-0.1811532973 \cdot 10^4$	$-0.1811533744 \cdot 10^4$
7	$-0.7953732143 \cdot 10^4$	$0.7954089807 \cdot 10^4$	$0.7954089068 \cdot 10^4$	$0.7954089765 \cdot 10^4$
8	$0.3544904563 \cdot 10^5$	$-0.3544868723 \cdot 10^5$	$-0.3544868703 \cdot 10^5$	$-0.3544868636 \cdot 10^5$
9	$-0.1598634544 \cdot 10^6$	$0.1598638127 \cdot 10^6$	$0.1598638125 \cdot 10^6$	$0.1598638127 \cdot 10^6$
10	$0.7279206365 \cdot 10^6$	$-0.7279202782 \cdot 10^6$	$-0.7279202781 \cdot 10^6$	$-0.7279202782 \cdot 10^6$

z are then expanded, yielding predictions for the next series coefficients that are exact rational numbers. Only in the final step, the predictions for the next series coefficients are converted to floating point numbers in order to improve readability:

$$\mathcal{A}_6^{(0)} = \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142857137\, z^{13} + 0.06666666629\, z^{14}$$
$$- 0.06249999856\, z^{15} + 0.05882352524\, z^{16} + O\!\left(z^{17}\right), \qquad (5.7a)$$

$$\epsilon_{12}^{(0)} = \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142854717\, z^{13} + 0.06666649774\, z^{14}$$
$$- 0.06249934843\, z^{15} + 0.05882168762\, z^{16} + O\!\left(z^{17}\right), \qquad (5.7b)$$

$$\mathcal{J}_4^{(0)} = \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142857148\, z^{13} + 0.06666666684\, z^{14}$$
$$- 0.06249999986\, z^{15} + 0.05882352708\, z^{16} + O\!\left(z^{17}\right), \qquad (5.7c)$$

$$\frac{\ln(1+z)}{z} = \sum_{m=0}^{12} \frac{(-z)^m}{m+1} - 0.07142857143\, z^{13} + 0.06666666667\, z^{14}$$
$$- 0.06250000000\, z^{15} + 0.05882352941\, z^{16} + O\!\left(z^{17}\right). \qquad (5.7d)$$

The accuracy of the prediction results in (5.7) is quite remarkable. The coefficients $\gamma_m = (-1)^m/(m+1)$ with $0 \le m \le 12$ are the only information that was used for the construction of the transformation terms $z^{13}\Phi_6^{(0)}(z)$, $z^{13}\varphi_{12}^{(0)}(z)$, and $z^{13}\Psi_4^{(0)}$, which were expanded to yield the

results in (5.7). The accuracy of the approximations to the next four coefficients should suffice for many practical applications.

As in all other application, Wynn's epsilon algorithm is in (5.7) slightly but significantly less effective than Aitken's iterated Δ^2 process and Brezinski's iterated theta algorithm.

Instead of computing the transformation terms $z^{13}\Phi_6^{(0)}(z)$, $z^{13}\varphi_{12}^{(0)}(z)$, and $z^{13}\Psi_4^{(0)}$, it is of course also possible to compute $\mathcal{A}_6^{(0)}$, $\epsilon_{12}^{(0)}$, and $\mathcal{J}_4^{(0)}$ directly via their defining recursive schemes, and to expand the resulting rational expressions with a symbolic system like Maple. This would lead to the same results. However, in order to extract the partial sum $\sum_{m=0}^{12}(-z)^m/(m+1)$ from the rational approximants $\mathcal{A}_6^{(0)}$, $\epsilon_{12}^{(0)}$, and $\mathcal{J}_4^{(0)}$, one would have to compute their 12-th order derivatives, and only the next derivatives would produce predictions to unknown series coefficients. Thus, this approach can easily become very expensive. In contrast, the use of the transformation terms requires only low order derivatives of rational expressions.

If only the prediction of a single unknown term is to be done, then it is of course much more efficient to use the recursive schemes (2.23), (3.17), and (4.21). The input data of these recursive schemes are the coefficients of the series to be transformed, and no differentiations have to be done.

6   Summary and Conclusions

As already mentioned in Section 1, it has become customary in certain branches of theoretical physics to use Padé approximants to make predictions for the leading unknown coefficients of strongly divergent perturbation expansions. This can be done by constructing symbolic expressions for Padé approximants from the known coefficients of the perturbation series. A Taylor expansion of sufficiently high order of such a Padé approximants then produces the predictions for the series coefficients which were not used for the construction of the Padé approximant. The Taylor expansion of the symbolic expression can be done comparatively easily with the help of powerful computer algebra systems like Maple or Mathematica, which are now commercially available for a wide range of computers.

It is the purpose of this article to overcome two principal shortcomings of the approach sketched above: Firstly, it is not necessary to rely entirely on the symbolic capabilities of computers. Instead, it is possible to construct recursive schemes, which either facilitate considerably the symbolic tasks computers have to perform, or which permit a straightforward computation of the prediction for the leading unknown coefficient. Secondly, it is possible to use instead of Padé approximants other sequence transformations, as proposed by Sidi and Levin [85] and Brezinski [18]. It was shown in [105] that this may lead to more accurate predictions.

In this article, the prediction properties of Aitken's iterated Δ^2 process, Wynn's epsilon algorithm, and Brezinski's iterated theta algorithm are studied.

As is well known [5, 8], a Padé approximant can be considered to be the solution of a system of linear equations for the coefficients of its numerator and denominator polynomials. If this system of linear equations has a solution, then it is automatically guaranteed that the Padé approximant satisfies the accuracy-through-order relationship (1.6). In the case of other

sequence transformations, the situation is usually much more difficult. They are usually not defined as solutions of systems of linear equations, but via (complicated) nonlinear recursive schemes.

Since accuracy-through-order relationships of the type of (1.6) play a very important role for the understanding of the prediction properties of sequence transformations, it was necessary to derive accuracy-through-order relationships for Aitken's iterated Δ^2 process, Wynn's epsilon algorithm, and Brezinski's iterated theta algorithm on the basis of their defining recursive schemes.

Unfortunately, the defining recursive schemes (2.4), (3.1), and (4.3) are not suited for a construction of accuracy-through-order relationships. They first had to be modified appropriately, yielding the mathematically equivalent recursive schemes (2.11), (3.8), and (4.11).

These alternative recursive schemes were the starting point for the derivation of the accuracy-through-order relationships (2.13), (3.9), and (4.13) and the corresponding recursive schemes (2.14), (3.9), and (4.14) for the transformation error terms. These relationships describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\epsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the function $f(z)$ which is to be approximated.

With the help of these accuracy-through-order relationships, a second group of results could be derived – (2.19), (3.14), and (4.18) and the corresponding recursive schemes (2.20), (3.15), and (4.19) – which describe how the rational approximants $\mathcal{A}_k^{(n)}$, $\epsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ differ from the partial sums which were used for their construction. These differences are expressed by the terms $z^{n+2k+1}\Phi_k^{(n)}(z)$, $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$, and $z^{n+3k+1}\Psi_k^{(n)}(z)$ which can be computed via the recursive schemes (2.20), (3.15), and (4.19).

The predictions for the leading unknown series coefficients can be obtained by expanding symbolic expressions for these transformation terms. The advantage of this approach is that the partial sums, which are used for the construction of the rational approximants $\mathcal{A}_k^{(n)}$, $\epsilon_{2k}^{(n)}$, and $\mathcal{J}_k^{(n)}$ as well as of the transformation terms $z^{n+2k+1}\Phi_k^{(n)}(z)$, $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$, and $z^{n+3k+1}\Psi_k^{(n)}(z)$, are already explicitly separated. Consequently, only derivatives of low order have to be computed. Moreover, the predictions for the leading unknown series coefficient can be computed conveniently via the recursive schemes (2.23), (3.17), and (4.21). In this way, it is neither necessary to construct symbolic expressions nor to differentiate them.

Finally, in Section 5 some applications of the new results were presented. In all applications of this article, Wynn's epsilon algorithm was found to be less effective than Aitken's iterated Δ^2 process or Brezinski's iterated theta algorithm. Of course, it remains to be seen whether this observation is specific for the infinite series (5.2) for $\ln(1+z)/z$, which was used as the test system, or whether it is actually more generally valid. Nevertheless, the results presented in Section 5 provide further evidence that suitably chosen sequence transformations may indeed be more effective than Padé approximants. Consequently, one should not assume that Padé approximants produce by default the best results in convergence acceleration and summation processes, and it may well be worth while to investigate whether sequence transformations can be found which are better adapted to the problem under consideration.

Acknowledgments

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