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The epsilon algorithm and related topics

P.R. Graves-Morris[a,*], D.E. Roberts[b], A. Salam[c]

[a]School of Computing and Mathematics, University of Bradford, Bradford, West Yorkshire BD7 1DP, UK
[b]Department of Mathematics, Napier University, Colinton Road, Edinburgh, EH14 1DJ Scotland, UK
[c]Laboratoire de Mathématiques Pures et Appliquées, Université du Littoral, BP 699, 62228 Calais, France

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Abstract

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

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1. Introduction

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

* Corresponding author.
E-mail address: p.r.graves-morris@bradford.ac.uk (P.R. Graves-Morris).

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

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

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

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

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

The importance of studying the vector epsilon algorithm lies partly in its potential [20] for application to the acceleration of convergence of iterative solution of discretised PDEs. For example, Gauss–Seidel iteration generates sequences of vectors which often converge too slowly to be useful. SOR, multigrid and Lanczos methods are alternative approaches to the problem which are currently popular, but the success of the techniques like CGS and LTPMs (see [31] for an explanation of the techniques and the acronyms) indicates the need for continuing research into numerical methods for the acceleration of convergence of vector-valued sequences.

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

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

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

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

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

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

2. The epsilon algorithm

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

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

and it comprises the following initialisation and iterative phases:

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

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

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

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

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

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

$$
\begin{array}{ccccc}
 & s_0 & & & \\
0 & & \varepsilon_1^{(0)} & & \\
 & s_1 & & \varepsilon_2^{(0)} & \\
0 & & \varepsilon_1^{(1)} & & \ddots \\
 & s_2 & & \varepsilon_2^{(1)} & \\
0 & & \varepsilon_1^{(2)} & & \\
 & s_3 & & \varepsilon_2^{(2)} & \\
0 & & \vdots & & \ddots \\
 & \vdots & & &
\end{array}
\qquad\qquad
\begin{array}{cccccc}
 & 4\cdot 000 & & & & \\
0 & & -0\cdot 75 & & & \\
 & 2\cdot 667 & & 3\cdot 167 & & \\
0 & & 1\cdot 25 & & -28\cdot 75 & \\
 & 3\cdot 467 & & 3\cdot 133 & & 3\cdot 142 \\
0 & & -1\cdot 75 & & 82\cdot 25 & \\
 & 2\cdot 895 & & 3\cdot 145 & & \\
0 & & 2\cdot 25 & & &
\end{array}
$$

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

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

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

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

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

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

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

its sections are defined by

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

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

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

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

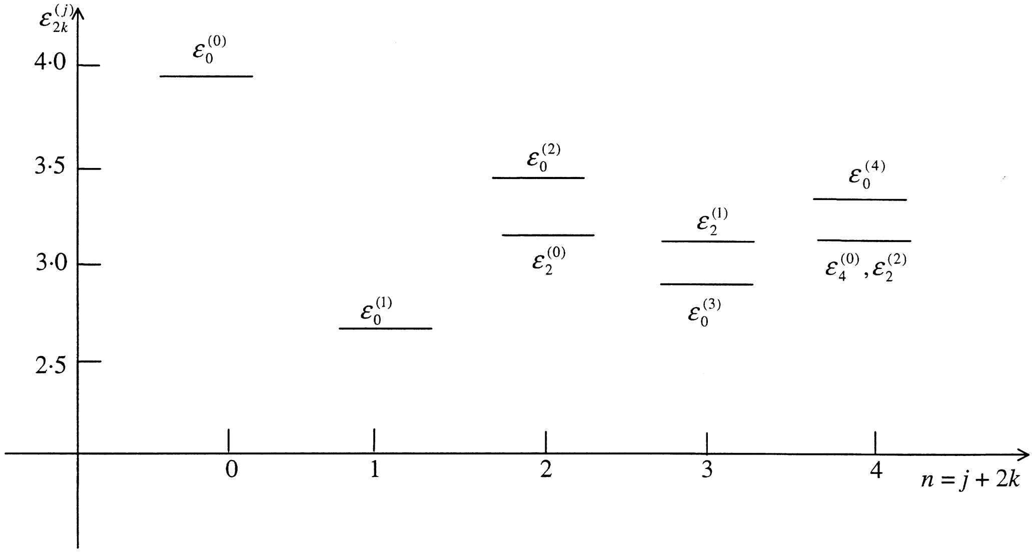

Fig. 2. Values of $\varepsilon_{2k}^{(j)}$ for Example 2.1, showing the convergence rate of the epsilon algorithm using $n+1 = 1,2,3,4,5$ terms of the given sequence.

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

$$f(z) = c_0 + c_1 z + c_2 z^2 + \cdots, \tag{2.8}$$

the rational function

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

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

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

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

(iii) $B(0) \neq 0.$ (2.12)

The Baker condition

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

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

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

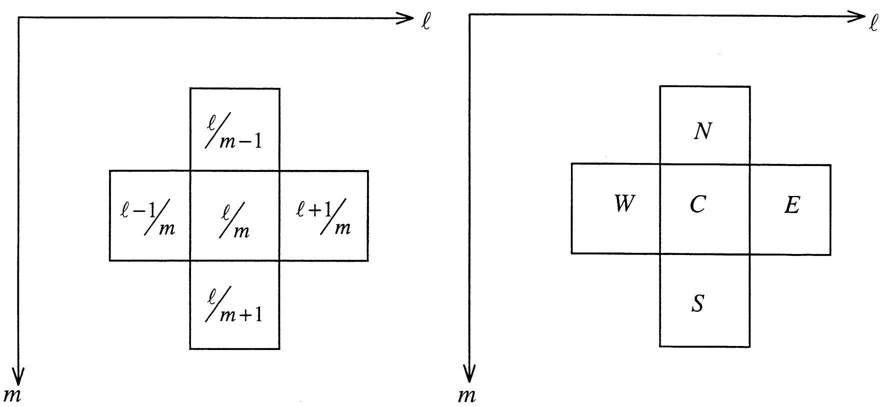

Fig. 3. Relative location of Padé approximants.

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

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

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

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

and then we find that

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

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

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

These approximants satisfy a five-point star identity,

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

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

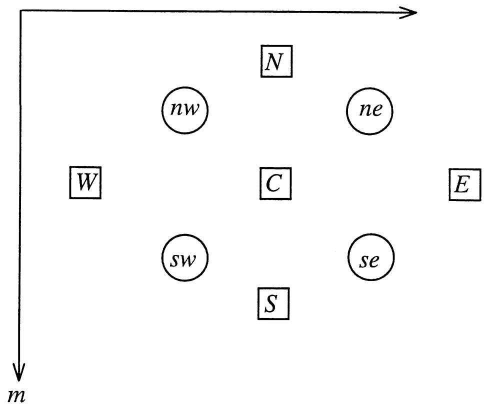

Fig. 4. Some artificial entries in the Padé table are shown circled.

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

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

and by

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

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

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

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

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

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

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

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

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

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

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

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

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

Example 2.2. We truncate (2.21) after a_2 and obtain

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

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

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

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

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

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

and the recursion is

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

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

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

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

where $[\,\cdot\,]$ represents the integer part function and the Baker normalisation is built in:

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

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

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

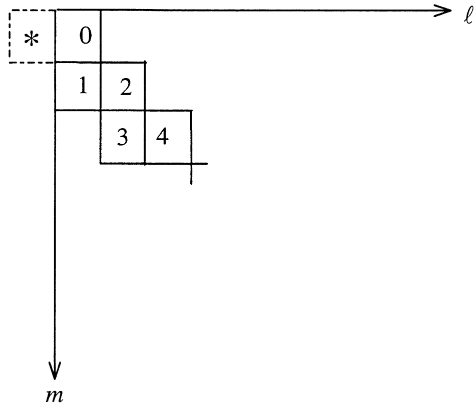

Fig. 5. A staircase sequence of approximants indexed by i, as in (2.27).

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

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

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

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

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

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

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

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

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

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

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

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

if

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

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

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

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

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

3. The vector epsilon algorithm

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

$$\boldsymbol{S} = (\boldsymbol{s}_0, \boldsymbol{s}_1, \boldsymbol{s}_2, \ldots : \boldsymbol{s}_i \in \mathbb{C}^d), \tag{3.1}$$

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

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

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

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

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

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

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

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

−0·10		
1·50		
0·59	0·96	
2·35	1·58	
1·43	0·57	1·00
2·08	1·44	1·00
1·80	0·40	1·00
1·11	0·76	1·00
1·54	0·90	1·00
0·26	0·57	1·00
0·95	1·16	⋮
0·09	0·64	
0·51	⋮	
0·60		
⋮		

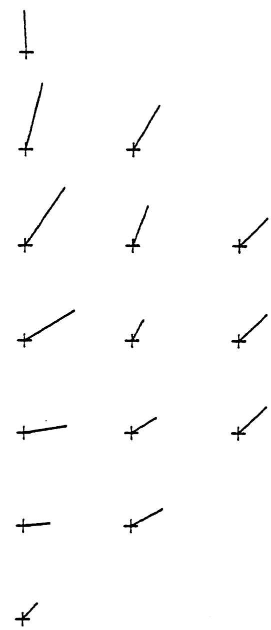

Fig. 6. Columns $k=0,2$ and 4 of the vector epsilon table for Example 3.1 are shown numerically and graphically.

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

Example 3.1. The sequence $\boldsymbol{S}$ is initialised by

$$\boldsymbol{s}_0 := \boldsymbol{b} := (-0.1, 1.5)^{\mathrm{T}} \tag{3.6}$$

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

$$\boldsymbol{s}_{j+1} := \boldsymbol{b} + G\boldsymbol{s}_j, \quad j = 0, 1, 2, \ldots \tag{3.7}$$

with

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

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

Notice that

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

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

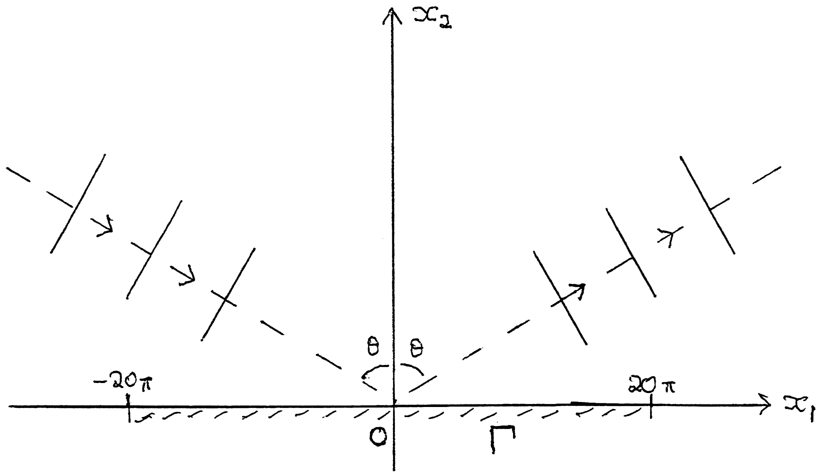

Fig. 7. Schematic view of the two components of $u_1(\boldsymbol{x})$ and the boundary Γ on the x_1-axis.

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

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

$$u(\boldsymbol{x}) = u_1(\boldsymbol{x}) + \mathrm{i}k \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})[\beta(\boldsymbol{y}) - 1]u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \tag{3.9}$$

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

$$u_1(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k(x_1 \sin\theta - x_2 \cos\theta)} + R.\mathrm{e}^{\mathrm{i}k(x_1 \sin\theta + x_2 \cos\theta)} \tag{3.10}$$

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

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

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

$$\frac{\partial u_1}{\partial x_2} = -\mathrm{i}ku_1 \quad \text{and} \quad \frac{\partial u}{\partial x_2} = -\mathrm{i}k\beta u \quad \text{on } \Gamma. \tag{3.12}$$

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

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

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

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

$$\begin{aligned}
\varepsilon_0^{(12)}&=[\,..,-\mathbf{0.36}843+\mathbf{0.4}4072\mathrm{i},\ldots,-\mathbf{0.145}07+\mathbf{0.5}5796\mathrm{i},\,..],\\
\varepsilon_2^{(10)}&=[\,..,-\mathbf{0.363}33+\mathbf{0.45}614\mathrm{i},\ldots,-\mathbf{0.1456}5+\mathbf{0.563}42\mathrm{i},\,..],\\
\varepsilon_4^{(8)}&=[\,..,-\mathbf{0.36341}+\mathbf{0.4558}2\mathrm{i},\ldots,-\mathbf{0.1456}8+\mathbf{0.5631}2\mathrm{i},\,..],\\
\varepsilon_6^{(6)}&=[\,..,-\mathbf{0.36341}+\mathbf{0.45583}\mathrm{i},\ldots,-\mathbf{0.14569}+\mathbf{0.56311}\mathrm{i},\,..],\\
\varepsilon_8^{(4)}&=[\,..,-\mathbf{0.36341}+\mathbf{0.45583}\mathrm{i},\ldots,-\mathbf{0.14569}+\mathbf{0.56311}\mathrm{i},\,..],
\end{aligned}$$

where the converged figures are shown in bold face.

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

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

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

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

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

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

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

From the given sequence $\boldsymbol{S} = (\boldsymbol{s}_i, i = 0, 1, 2, \ldots, : \boldsymbol{s}_i \in \mathbb{C}^d)$, we form the series coefficients

$$\boldsymbol{c}_0 := \boldsymbol{s}_0, \quad \boldsymbol{c}_i := \boldsymbol{s}_i - \boldsymbol{s}_{i-1}, \qquad i = 1, 2, 3, \ldots \tag{3.15}$$

and the associated generating function

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

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

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

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

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

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

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

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

$$w_3 = \alpha w_1 + \beta w_2 \in \mathscr{V}_{\mathbb{C}} \tag{3.20}$$

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

$$f(z) = c_0 + c_1 z + c_2 z^2 + \cdots \in \mathscr{V}_{\mathbb{C}}[[z]]. \tag{3.21}$$

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

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

then

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

Hence (3.18) and (3.19) imply that

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

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

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

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

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

where

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

so that w^{-1} is the image of $\boldsymbol{w}^{-1}$ as defined by (3.5). Thus (3.19) specifies an isomorphism between

(i) the space $\mathbb{C}^d$, having representative element

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

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

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

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

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

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

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

Lemma 3.3. *Let $w, t \in \mathscr{V}_{\mathbb{C}}$ be the images of $\boldsymbol{w} = \boldsymbol{x} + \mathrm{i}\boldsymbol{y}$, $\boldsymbol{t} = \boldsymbol{u} + \mathrm{i}\boldsymbol{v} \in \mathbb{C}^d$. Then*

(i) $t\tilde{w} + w\tilde{t} = 2\,\mathrm{Re}(\boldsymbol{w}^{\mathrm{H}}\boldsymbol{t})I \in \mathscr{S}$, (3.27)

(ii) $w\tilde{t}w = 2w\,\mathrm{Re}(\boldsymbol{w}^{\mathrm{H}}\boldsymbol{t}) - t||\boldsymbol{w}||^2 \in \mathscr{V}_{\mathbb{C}}$. (3.28)

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

$$t\tilde{w} + w\tilde{t} = \sum_{i=1}^{d}\sum_{j=1}^{d}(u_iE_i + v_iF_i)(x_jE_j - y_jF_j) + (x_jE_j + y_jF_j)(u_iE_i - v_iF_i)$$
$$= (\boldsymbol{u}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{y})I = 2\,\mathrm{Re}(\boldsymbol{w}^{\mathrm{H}}\boldsymbol{t})I$$

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

$$F_iE_j - E_jF_i = 0, \quad F_iF_j + F_jF_i = -2\delta_{ij}I.$$

For part (ii), we simply note that

$$w\tilde{t}w = w(\tilde{t}w + \tilde{w}t) - w\tilde{w}t. \qquad \Box$$

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

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

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

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

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

$$e_{2j+1} \in \mathscr{V}_{\mathrm{C}}. \tag{3.31}$$

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

$$e_{2j+1} = \begin{vmatrix} c_0 & \cdots & c_{j+1} \\ \vdots & & \vdots \\ c_{j+1} & \cdots & c_{2j+2} \end{vmatrix}_{\ell}. \tag{3.31b}$$

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

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

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

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

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

Proceeding with the elimination in (3.29), we obtain

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

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

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

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

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

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

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

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

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

These definitions are initialised with

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

Example 3.5.

$$A_1(z) = c_0, \quad B_1(z) = I - z c_0^{-1} c_1, \quad e_1 = c_2 - c_1 c_0^{-1} c_1,$$

$$D_1(z) = c_1^{-1} - z \tilde{c}_1 \tilde{c}_0^{-1} c_1^{-1}. \tag{3.39}$$

Lemma 3.6.

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

Proof. See (3.35) and (3.38). □

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

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

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

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

(iv) $e_j \in \mathscr{V}_C.$ (3.44)

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

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

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

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

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

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

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

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

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

Part (iv): By definition (3.36),

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

For $J > 0$, we use

$$A_0^{(J)}(z) = \sum_{i=0}^{J} c_i z^i, \quad B_0^{(J)}(z) = I, \quad e_0^{(J)} = c_{J+1},$$

$$A_{-1}^{(J)}(z) = \sum_{i=0}^{J-1} c_i z^i, \quad B_{-1}^{(J)}(z) = I, \quad e_{-1}^{(J)} = c_J, \tag{3.50}$$

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

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

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

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

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

corresponding to

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

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

Then, for $J<0$,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Similarly, we find that

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

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

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

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

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

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

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

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

(ii) $Q^{[n/2k]}(z)$ is a factor of $\boldsymbol{P}^{[n/2k]}(z).\boldsymbol{P}^{[n/2k]*}(z),$ (3.63)

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

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

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

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

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

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

Proof. Suppose that

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

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

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

From (3.63) and (3.65) we find that

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

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

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

$$\boldsymbol{f}(z) = \boldsymbol{a}(z)b^*(z)/b(z)b^*(z)$$

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

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

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

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

$$\varepsilon_{2k}^{(j)} = \boldsymbol{s}_\infty, \quad j = 0, 1, 2, \ldots \tag{3.69}$$

provided that zero divisors are not encountered in the construction.

The previous theorem is a statement about exact results in the column of index $2k$ in the vector epsilon table. This column corresponds to the row sequence of GIPAs of type $[n/2k]$ for $\boldsymbol{f}(z)$, evaluated at $z=1$. If the given vector sequence $\boldsymbol{S}$ is nearly, but not exactly, generalized geometric, we model this situation by supposing that its generating function $\boldsymbol{f}(z)$ is analytic in the closed unit disk $\bar{D}$, except for k poles in $D := \{z \colon |z| < 1\}$. This hypothesis ensures that $\boldsymbol{f}(z)$ is analytic at $z=1$, and it is sufficiently strong to guarantee convergence of the column of index $2k$ in the vector epsilon table. There are several convergence theorems of this type [28–30,39]. It is important to note that any row convergence theorem for generalised inverse vector-valued Padé approximants has immediate consequences as a convergence result for a column of the vector epsilon table.

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

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

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

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

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

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

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

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

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

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

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

4. Vector-valued continued fractions and vector orthogonal polynomials

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

$$\boldsymbol{f}(z) = \boldsymbol{c}_0 + \boldsymbol{c}_1 z + \boldsymbol{c}_2 z^2 + \cdots \tag{4.1}$$

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

$$f(z) = c_0 + c_1 z + c_2 z^2 + \cdots \tag{4.2}$$

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

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

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

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

and the corresponding element of the vector epsilon table is

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

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

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

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

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

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

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

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

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

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

$$
\begin{array}{ccc}
 & \alpha_m^{(J)} & \\
\beta_{m-1}^{(J+1)} & & \beta_m^{(J)} \\
 & \alpha_m^{(J+1)} &
\end{array}
\qquad\qquad
\begin{array}{ccc}
 & \beta_m^{(J)} & \\
\alpha_m^{(J+1)} & & \alpha_{m+1}^{(J)} \\
 & \beta_m^{(J+1)} &
\end{array}
$$

Rule (4.6) **Rule (4.7)**

Fig. 8.

Proof. First, the identity

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

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

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

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

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

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

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

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

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

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

and accuracy-through-order is expressed by

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

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

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

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

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

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

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

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

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

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

the error vectors obey the identity

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

for $J \geqslant 0$ *and* $i \geqslant 0$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

corresponding to the same compass identity amongst designants.

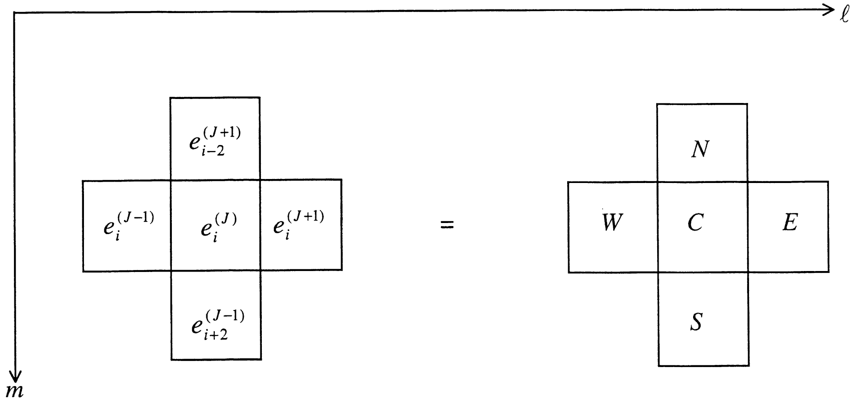

Fig. 9. Position of error vectors obeying the cross-rule.

Reverting to the normalisation of (3.64) with $q_\Omega(0) = I$ and $Q_\Omega(0) = 1$, we note that formula (3.28) is required to convert (4.22) to a usable relation amongst vectors $\boldsymbol{e}_\Omega \in \mathbb{C}^d$. We find that

$$\boldsymbol{e}_S = \boldsymbol{e}_E - |\boldsymbol{e}_C|^2 \left[\frac{\boldsymbol{e}_N}{|\boldsymbol{e}_N|^2} - \frac{\boldsymbol{e}_W}{|\boldsymbol{e}_W|^2} \right] + 2\boldsymbol{e}_C \operatorname{Re} \left[\boldsymbol{e}_C^{\mathrm{H}} \left(\frac{\boldsymbol{e}_N}{|\boldsymbol{e}_N|^2} - \frac{\boldsymbol{e}_W}{|\boldsymbol{e}_W|^2} \right) \right]$$

and this formula is computationally executable.

Implementation of this formula enables the calculation of the vectors $\boldsymbol{e}_\Omega$ in $\mathbb{C}^d$ in a rowwise fashion (see Fig. 9). For the case of vector-valued meromorphic functions of the type described following (3.69) it is shown in [40] that asymptotic (i.e., as J tends to infinity) results similar to the scalar case are valid, with an interesting interpretation for the behaviour of the vectors $\boldsymbol{e}_i^{(J)}$ as J tends to infinity. It is also shown in [40] that, as in the scalar case, the above procedure is numerically unstable, while a column-by-column computation retains stability – i.e., (4.22) is used to evaluate $\boldsymbol{e}_E$. There are also considerations of underflow and overflow which can be dealt with by a mild adaptation of the cross-rule.

Orthogonal polynomials lie at the heart of many approximation methods. In this context, the orthogonal polynomials are operators $\pi_i(\xi) \in \mathscr{A}[\xi]$, and they are defined using the functionals $c\{\cdot\}$ and $\boldsymbol{c}\{\cdot\}$. These functionals are defined by their action on monomials:

$$c\{\xi^i\} = c_i, \quad \boldsymbol{c}\{\xi^i\} = \boldsymbol{c}_i. \tag{4.25}$$

By linearity, we can normally define monic vector orthogonal polynomials by $\pi_0(\xi) = I$ and, for $i = 1, 2, 3, \ldots$, by

$$c\{\pi_i(\xi)\xi^j\} = 0, \quad j = 0, 1, \ldots, i-1. \tag{4.26}$$

The connection with the denominator polynomials (3.35) is

Theorem 4.3. *For* $i = 0, 1, 2, \ldots$

$$\pi_i(\xi) = \xi^i B_{2i-1}(\xi^{-1}).$$

Proof. Since $B_{2i-1}(z)$ is an operator polynomial of degree i, so is $\pi_i(\xi)$. Moreover, for $j=0,1,\ldots,i-1$,

$$c\{\xi^j\pi_i(\xi)\}=c\{\xi^{i+j}B_{2i-1}(\xi^{-1})\}=\sum_{\ell=0}^{i}c\{\xi^{i+j-\ell}B_\ell^{(2i-1)}\}=\sum_{\ell=0}^{i}c_{i+j-\ell}B_\ell^{(2i-1)}$$

$$=[f(z)B_{2i-1}(z)]_{i+j}=0$$

as is required for (4.26). □

This theorem establishes an equivalence between approximation methods based on vector orthogonal polynomials and those based on vector Padé approximation. To take account of noncommutativity, more care is needed over the issue of linearity with respect to multipliers from $\mathscr{A}$ than is shown in (4.26). Much fuller accounts, using variants of (4.26), are given by Roberts [41] and Salam [44,45].

In this section, we have focussed on the construction and properties of the continued fractions associated with the leading diagonal sequence of vector Padé approximants. When these approximants are evaluated at $z=1$, they equal $\varepsilon_{2k}^{(0)}$, the entries on the leading diagonal of the vector epsilon table. These entries are our natural first choice for use in the acceleration of convergence of a sequence of vectors.

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