VECTOR PADE APPROXIMANTS

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Abstract

We consider the construction of rational approximations to given power series whose coefficients are vectors. The approximants are in the form of vector-valued continued fractions which may be used to obtain vector Padé approximants using recurrence relations. Algorithms for the determination of these fractions have been established using Clifford algebras. We devise new algorithms based on these which involve only vectors and scalars — a desirable characteristic for computations involving vectors of large dimension.Finally, we present a novel use of Clifford algebras by suggesting a definition of approximant which reflects more faithfully the singularities of the given function.

1 Introduction

This paper illustrates some of the advantages of Clifford algebras in the construction of rational approximants to vector-valued functions. The algebraic context allows a development of the vector theory which parallels that of the scalar, so that proofs of theorems and algorithms valid in the scalar case may be carried over to the vector version. Baker and Graves-Morris provide an introduction to the usual theory of Padé approximants and some generalisations. In particular, we focus attention on the use of two related algorithms — viz the Viskovatov and Modified Euclidean to derive *corresponding* continued fraction representations of the given function. We are then able to establish certain properties which are enjoyed by all vector Padé approximants.

Since, in many applications, the dimension of the vectors can be quite large — in some instances of several thousand — an approach is sought which allows the aforementioned operations to be performed using scalars and vectors only. [N.B. Matrix representations of $C\ell_n$ involve dimensions of the order $2^{n/2}$.] We demonstrate how this may be achieved by taking advantage of the algebraic structure of $C\ell_n$.

In section five, our interest centres around the application of rational approximation theory to the acceleration of the convergence of vector sequences. In this context the vector ϵ -algorithm, introduced by Wynn in 1962, has been employed to calculate vector Padé approximants. Indeed, it was McLeod(1971) and Wynn(1968) who first used Clifford numbers in an attempt to build an algebraic description of the vector ϵ -algorithm. However, the vector Padé approximant to the generating function corresponding to a sequence yields too many singularities. We show how this may be remedied, in general, by recourse to the Clifford description of the denominator polynomial, which, together with the results of a particular convergence theorem, suggests a natural definition as an alternative to the usual Padé version. For the simplest non-trivial case the new approximant provides an acceleration procedure essentially that of a successful vector version of the well known Aitken δ^2 method.

2 Vector Padé Approximants

We consider a vector-valued function, $\mathbf{f}: \mathbb{C} \to \mathbb{C}^n$, which has a MacLaurin series

$$\mathbf{f}(z) = \mathbf{c}_0 + z\mathbf{c}_1 + z^2\mathbf{c}_2 + \dots, \quad z \in \mathbb{C}, \quad \mathbf{c}_i \in \mathbb{R}^n, \quad i = 0, 1, \dots$$
(2.1)

valid in some neighbourhood of the origin. In this paper we restrict attention to *real vectors*, which is the more common situation in practical applications. However, for a discussion of the case of complex vector coefficients the reader is referred to the author's 1995 paper and to Graves-Morris *et al.*, 1994. The right-handed [l/m] vector Padé approximant (VPA) to $\mathbf{f}(z)$, if it exists, is defined by

$$[l/m](z) := p^{[l/m]}(z)[q^{[l/m]}(z)]^{-1}$$
(2.2)

for which

$$[l/m](z) - \mathbf{f}(z) = O(z^{l+m+1})$$
(2.3)

where $p^{[l/m]}(z)$ and $q^{[l/m]}(z)$ are polynomials in $z \in \mathbb{C}$ over $C\ell_n$ of maximum degrees l and m respectively. These approximants share many of the properties enjoyed by the scalar version; in particular, for given l and m, [l/m](z) is unique for an explanation and further discussion see Roberts (1990). They may be arrayed in a two-dimensional table as in Fig.1. Assuming that $q^{[l/m]}(0)$ is invertible then, on multiplying (2.3) by $q^{[l/m]}(z)$ from the right, we obtain

$$p^{[l/m]}(z) - \mathbf{f}(z)q^{[l/m]}(z) = O(z^{l+m+1})$$
(2.4)

[0/0]	[1/0]	[2/0]	
[0/1]	[1/1]	[2/1]	
[0/2]	[1/2]	[2/2]	
:	:	:	

Figure 1: The Vector Padé Table

which yields a system of (l + m + 1) linear equations in the (l + m + 2) unknown coefficients of $p^{[l/m]}(z)$ and $q^{[l/m]}(z)$. If we set

$$p^{[l/m]}(z) = a_0 + a_1 z + a_2 z^2 + \dots + a_{l-1} z^{l-1} + a_l z^l$$

and

$$q^{[l/m]}(z) = b_0 + b_1 z + b_2 z^2 + \dots + b_{m-1} z^{m-1} + b_m z^m$$

where $a_i, b_j \in C\ell_n$ for $i = 0, 1, \dots, l$ and $j = 0, 1, \dots, m$ then, on considering the powers of z up to the $(l+m)^{th}$, we obtain

$$\left. \begin{array}{l} a_{0} = \mathbf{c}_{0}b_{0} \\ a_{1} = \mathbf{c}_{1}b_{0} + \mathbf{c}_{0}b_{1} \\ a_{2} = \mathbf{c}_{2}b_{0} + \mathbf{c}_{1}b_{1} + \mathbf{c}_{0}b_{2} \\ \vdots \\ a_{l} = \mathbf{c}_{l}b_{0} + \mathbf{c}_{l-1}b_{1} + \dots + \mathbf{c}_{l-m}b_{m} \end{array} \right\}$$

$$(2.5)$$

and

$$\left. \begin{array}{c} \mathbf{c}_{l+1}b_{0} + \mathbf{c}_{l}b_{1} + \mathbf{c}_{l-1}b_{2} + \dots + \mathbf{c}_{l-m+2}b_{m-1} + \mathbf{c}_{l-m+1}b_{m} = 0 \\ \mathbf{c}_{l+2}b_{0} + \mathbf{c}_{l+1}b_{1} + \mathbf{c}_{l}b_{2} + \dots + \mathbf{c}_{l-m+3}b_{m-1} + \mathbf{c}_{l-m+2}b_{m} = 0 \\ \vdots \\ \mathbf{c}_{l+m}b_{0} + \mathbf{c}_{l+m-1}b_{1} + \mathbf{c}_{l+m-2}b_{2} + \dots + \mathbf{c}_{l+1}b_{m-1} + \mathbf{c}_{l}b_{m} = 0 \end{array} \right\}$$

$$(2.6)$$

Example 1. Let m := 1 and adopt the Baker convention (see for example Baker *et al.* 1981) by setting $b_0 := \mathbf{e}_0$ in (2.6). Then we obtain $b_1 = -\mathbf{c}_l^{-1}\mathbf{c}_{l+1}$ thus yielding

$$q^{[l/1]}(z) = \mathbf{e}_0 - z\mathbf{c}_l^{-1}\mathbf{c}_{l+1}.$$
 (2.7)

The [l/1] vector Padé approximant is given by

$$\mathbf{c}_{0} + \mathbf{c}_{1}z + \mathbf{c}_{2}z^{2} + \dots + \mathbf{c}_{l-1}z^{l-1} + z^{l}\mathbf{c}_{l}[\mathbf{e}_{0} - z\mathbf{c}_{l}^{-1}\mathbf{c}_{l+1}]^{-1}$$
(2.8)

which may be verified by expanding the denominator using the binomial theorem.

Example 2. For m := 2 equations (2.6) become

$$\mathbf{c}_l b_1 + \mathbf{c}_{l-1} b_2 = -\mathbf{c}_{l+1} b_0$$

$$\mathbf{c}_{l+1}b_1 + \mathbf{c}_l b_2 = -\mathbf{c}_{l+2}b_0$$

If we eliminate b_1 from the second equation we obtain

$$\mathbf{\Delta}_l b_2 = [\mathbf{c}_l \mathbf{c}_{l+1}^{-1} \mathbf{c}_{l+2} - \mathbf{c}_{l+2}] b_0$$

where we define the vector

$$\mathbf{\Delta}_l := \mathbf{c}_{l-1} - \mathbf{c}_l \mathbf{c}_{l+1}^{-1} \mathbf{c}_l.$$

More generally, systems of linear equations whose coefficients do not commute may be solved using *designants* — of which Δ_l is an example. These were invented by Heyting in 1927 and first applied in the current context by Salam in 1993. From the above we have

$$b_{2} = \Delta_{l}^{-1} [\mathbf{c}_{l} \mathbf{c}_{l+1}^{-1} \mathbf{c}_{l+2} - \mathbf{c}_{l+1}] b_{1} = -\mathbf{c}_{l+1}^{-1} \mathbf{c}_{l} \Delta_{l}^{-1} [\mathbf{c}_{l-1} \mathbf{c}_{l}^{-1} \mathbf{c}_{l+2} - \mathbf{c}_{l+1}]$$

$$(2.9)$$

where b_0 is again taken to be the identity \mathbf{e}_0 . We may now construct the [l/2] denominator polynomial:

$$q^{[l/2]}(z) = \mathbf{e}_0 + b_1 z + b_2 z^2.$$
(2.10)

However, one may see that the resulting expression in terms of the series coefficients is rather cumbersome. Hence, a different approach to the computation of these approximants is desirable. The next section describes one based on continued fractions, which offers the advantage of recurrence relations for their evaluation.

3 Corresponding Vector Continued Fractions

In this section we consider the problem of expressing the given power series in the form of a continued fraction — as in equation (3.5). A common approach in the scalar context is Viskovatov's algorithm which dates from 1803-6. We develop this method for the non-degenerate case and, in the course of doing so, demonstrate the existence of the inverses necessary for its implementation.

Viskovatov's algorithm as formulated by Baker *et al.* may be adapted for noncommuting elements by constructing the identity

$$\left(\sum_{i=0}^{\infty} d_{k,i} z^{i}\right) \left(\sum_{i=0}^{\infty} d_{k+1,i} z^{i}\right)^{-1} = d_{k,0} (d_{k+1,0})^{-1} + z \left[\left(\sum_{i=0}^{\infty} d_{k+1,i} z^{i}\right) \left(\sum_{i=0}^{\infty} d_{k+2,i} z^{i}\right)^{-1}\right]^{-1} \right\}$$
(3.1)

where

$$d_{k+2,i} := d_{k,i+1} - [d_{k,0}(d_{k+1,0})^{-1}]d_{k+1,i+1} \quad \text{for } k, i = 0, 1 \cdots .$$
(3.2)

The application to the vector-valued power series (2.1) is achieved by setting

On defining

$$\boldsymbol{\pi}_k := d_{k,0} (d_{k+1,0})^{-1} \tag{3.4}$$

and using (3.1) repeatedly we obtain a continued fraction expansion of $\mathbf{f}(z)$,

$$\mathbf{f}(z) := \boldsymbol{\pi}_0 + z [\boldsymbol{\pi}_1 + z [\boldsymbol{\pi}_2 + \cdots]^{-1}]^{-1}$$
(3.5)

The first few elements are

$$\boldsymbol{\pi}_0 := \mathbf{c}_0, \ \boldsymbol{\pi}_1 := \mathbf{c}_1^{-1}, \ \boldsymbol{\pi}_2 := -\mathbf{c}_1 \mathbf{c}_2^{-1} \mathbf{c}_1, \ \boldsymbol{\pi}_3 := [\mathbf{c}_1 \mathbf{c}_2^{-1} \mathbf{c}_3 \mathbf{c}_2^{-1} \mathbf{c}_1 - \mathbf{c}_1]^{-1}, \cdots$$

which are all vectors in \mathbb{R}^n . However, we also require expressions for the $d_{k,i}$, viz

$$d_{2,i} := \mathbf{c}_{i+1}, \ d_{3,i} := -\mathbf{c}_1^{-1}\mathbf{c}_{i+2}, \ d_{4,i} := \mathbf{c}_{i+2} - \mathbf{c}_1\mathbf{c}_2^{-1}\mathbf{c}_{i+3}, \cdots$$

- which become increasingly more complicated. In order to develop a version of this algorithm which may be implemented using vectors and scalars only we proceed as follows. Define

$$S_k(z) := \sum_{i=0}^{\infty} d_{k,i} z^i$$

so that (3.2) and (3.4) become

$$S_{k+2}(z) := \frac{1}{z} [S_k(z) - \boldsymbol{\pi}_k S_{k+1}(z)]$$
(3.6)

$$\boldsymbol{\pi}_k := S_k(0)[S_{k+1}(0)]^{-1} \tag{3.7}$$

while the identity (3.1) now reads

$$S_k(z)[S_{k+1}(z)]^{-1} := \boldsymbol{\pi}_k + z[S_{k+1}(z)[S_{k+2}(z)]^{-1}]^{-1}$$
(3.8)

with

$$S_0(z) := \mathbf{f}(z) \text{ and } S_1(z) := \mathbf{e}_0$$
 (3.9)

replacing the initialization (3.3). If we further define

$$\mathbf{V}_{k+1}(z) := S_k(z)\widetilde{S_{k+1}}(z)$$
 and $u_k(z) := S_k(z)\widetilde{S_k}(z)$ for $k = 0, 1 \cdots$ (3.10)

then it is straightforward to prove by induction that $\mathbf{V}_{k+1}(z)$ is a real analytic vector function and $u_k(z)$ a real analytic function for $k = 0, 1 \cdots$. In fact, by considering $S_k(z)\widetilde{S_{k+1}}(z)$ and $S_{k+1}(z)\widetilde{S_{k+1}}(z)$, using (3.6) and (3.9) we may obtain

with the initializations

$$\mathbf{V}_1(z) := \mathbf{f}(z) \text{ and } u_0(z) := \mathbf{f}(z) \cdot \mathbf{f}(z) , \ u_1(z) := 1.$$
 (3.12)

We then have

$$\boldsymbol{\pi}_{k} = S_{k}(0)[S_{k+1}(0)]^{-1} = \frac{\mathbf{V}_{k+1}(0)}{u_{k+1}(0)}$$
(3.13)

- -

which is a vector in \mathbb{R}^n . In this section we assume non-degeneracy i.e. that $\mathbf{V}_k(0)$ is non-null for $k = 1, 2, \cdots$. Indeed, $[S_{k+1}(z)]^{-1}$ exists as a power series if $S_{k+1}(0) \in$ Γ_n which may be proved by induction using the definition of $\mathbf{V}_{k+1}(0)$ and the above assumption. We may then also conclude that $u_{k+1}(0)$ is non-zero which ensures the validity of (3.13).

In summary, the recurrence relations (3.11) with the initializations (3.12) form a version of Viskovatov's algorithm using only vectors and scalars, allowing the determination of the continued fraction elements of (3.5). We now prove that this fraction *corresponds* to the given power series, i.e. that the k^{th} convergent

$$\mathbf{C}_{k}(z) := \boldsymbol{\pi}_{0} + z[\boldsymbol{\pi}_{1} + z[\boldsymbol{\pi}_{2} + \dots + z[\boldsymbol{\pi}_{k}]^{-1} \cdots]^{-1}]^{-1}$$

satisfies the order condition

$$\mathbf{f}(z) - \mathbf{C}_k(z) = O(z^{k+1}). \tag{3.14}$$

From Roberts (1990), we have

$$\mathbf{C}_{k}(z) = p_{k}(z)[q_{k}(z)]^{-1}$$
(3.15)

where the polynomials $p_k(z), q_k(z)$, over $C\ell_n$ satisfy the recurrence relations

$$p_{k}(z) := p_{k-1}(z)\boldsymbol{\pi}_{k} + zp_{k-2}(z) \quad p_{-1}(z) := \mathbf{e}_{0}, \quad p_{0}(z) := \boldsymbol{\pi}_{0} q_{k}(z) := q_{k-1}(z)\boldsymbol{\pi}_{k} + zq_{k-2}(z) \quad q_{-1}(z) := 0, \quad q_{0}(z) := \mathbf{e}_{0}$$

$$(3.16)$$

It is straightforward to prove the following by induction

$$\mathbf{f}(z)q_k(z) - p_k(z) = (-1)^k z^{k+1} \widetilde{S_{k+2}}(z).$$
(3.17)

Assuming non-degeneracy we observe that (3.14) is then satisfied, since

$$q_k(0) = q_{k-1}(0) \boldsymbol{\pi}_k = \boldsymbol{\pi}_1 \boldsymbol{\pi}_2 \boldsymbol{\pi}_3 \cdots \boldsymbol{\pi}_k \neq 0$$

using (3.16). We may, in fact, go further and obtain the leading term on the right hand side of the order condition as follows. From (3.13) we have

$$S_{k+2}(0) = [\boldsymbol{\pi}_{k+1}]^{-1} S_{k+1}(0) = [\boldsymbol{\pi}_{k+1}]^{-1} [\boldsymbol{\pi}_{k}]^{-1} \cdots [\boldsymbol{\pi}_{1}]^{-1} = [\boldsymbol{\pi}_{1} \boldsymbol{\pi}_{2} \boldsymbol{\pi}_{3} \cdots \boldsymbol{\pi}_{k+1}]^{-1}$$

since $S_1(0) = \mathbf{e}_0$. Therefore,

$$\mathbf{f}(z)q_k(z) - p_k(z) = (-1)^k z^{k+1} [\boldsymbol{\pi}_{k+1} \boldsymbol{\pi}_k \cdots \boldsymbol{\pi}_2 \boldsymbol{\pi}_1]^{-1} + O(z^{k+2})$$

from which we obtain the symmetric result for the order condition (3.14)

$$\mathbf{f}(z) - p_k(z)[q_k(z)]^{-1} = (-1)^k z^{k+1} [q_k(0)\boldsymbol{\pi}_{k+1}\widetilde{q_k}(0)]^{-1} + O(z^{k+2})$$
$$= (-1)^k z^{k+1} [\boldsymbol{\pi}_1]^{-1} [\boldsymbol{\pi}_2]^{-1} \cdots [\boldsymbol{\pi}_k]^{-1} [\boldsymbol{\pi}_{k+1}]^{-1} [\boldsymbol{\pi}_k]^{-1} \cdots [\boldsymbol{\pi}_1]^{-1} + O(z^{k+2}).$$

The successive convergents of (3.5) yield the staircase sequence of vector Padé approximants $[0/0], [1/0], [1/1], [2/1], \cdots$.

4 The Modified Euclidean Algorithm

The Viskovatov algorithm may be adapted in the event of meeting degeneracies i.e. when, $\mathbf{V}_k(0)$ and hence $S_k(0)$ vanish. However, a closely related method which is *reliable* [see Baker *et al.* for a discussion of this characteristic] and generates *diagonal* approximants, is the modified Euclidean algorithm as presented by Graves-Morris and Roberts for the vector case. Here, we simply state this algorithm, which employs a different definition of $S_k(z)$ for positive k from that of Viskovatov, and refer the reader to the aforementioned paper for a detailed discussion and proof, which broadly uses the ideas of the previous section.

The aim is to generate a continued fraction which corresponds to the power series of $\mathbf{f}(z)$:

$$\mathbf{f}(z) = \boldsymbol{\pi}_0(z) + z^{\mu_1} [\boldsymbol{\pi}_1(z) + z^{\mu_2} [\boldsymbol{\pi}_2(z) + \cdots]^{-1}]^{-1}$$
(4.1)

in which each $\pi_i(z)$ is a vector-valued polynomial of degree ν_i and each μ_i is a positive integer. This is achieved by using (3.9) and repeatedly applying :

$$S_k(z)[S_{k+1}(z)]^{-1} := \boldsymbol{\pi}_k(z) + z^{\mu_{k+1}}[S_{k+1}(z)[S_{k+2}(z)]^{-1}]^{-1},$$

in which the integers μ_k and the polynomials $\pi_k(z)$ are provided by the modified Euclidean algorithm as follows.

We start by defining the quantities :

$$\pi_{0} := S_{0}(0)S_{1}(0)^{-1} = \mathbf{f}(0) \quad \nu_{0} := 0 \mu_{1} := O(S_{0}(z) - \boldsymbol{\pi}_{0}S_{1}(z)) \quad \nu_{1} := \mu_{1}$$

$$(4.2)$$

Then the recurrence scheme is implemented :

$$\begin{aligned}
S_{k+1}(z) &:= z^{-\mu_k} [S_{k-1}(z) - \boldsymbol{\pi}_{k-1} S_k(z)] \\ \boldsymbol{\pi}_k(z) &:= [S_k(z) S_{k+1}(z)^{-1}]_0^{\nu_k}, \end{aligned} \} \quad k := 1, 2, \cdots$$
(4.3)

$$\mu_{k+1} := O(S_k(z) - \pi_k(z)S_{k+1}(z)) \nu_{k+1} := \mu_{k+1} - \nu_k$$
 $k := 1, 2, \cdots$ (4.4)

employing the Nuttal notation for the Maclaurin section :

$$[\phi(z)]_0^k := \sum_{i=0}^k \phi_i z^i.$$

As a consequence of this construction $S_k(0) \in \Gamma_n$ for $k \geq 1$.

We implement this algorithm in such a way as to require scalar and vector functions only, by following the approach outlined in the previous section. Using the definitions (3.10) it may be demonstrated that, as before, $\mathbf{V}_k(z) \in \mathbb{C}^n$ and that $u_k(z) \in \mathbb{C}$. The first of the recurrence relations (4.3) is replaced by

$$\left. \begin{array}{l} \mathbf{V}_{k+2}(z) = z^{-\mu_{k+1}} [\mathbf{V}_{k+1}(z) - \boldsymbol{\pi}_{k}(z) u_{k+1}(z)] \\ u_{k+2}(z) = z^{-2\mu_{k+1}} [u_{k}(z) - 2\boldsymbol{\pi}_{k}(z) \cdot \mathbf{V}_{k+1}(z) + \boldsymbol{\pi}_{k}(z) \cdot \boldsymbol{\pi}_{k}(z) u_{k+1}(z)] \end{array} \right\}$$
(4.5)

while the second becomes

$$\boldsymbol{\pi}_{k}(z) := [\mathbf{V}_{k+1}(z)/u_{k+1}(z)]_{0}^{\nu_{k}}.$$
(4.6)

We note that synthetic division is not necessary to calculate $\pi_k(z)$. For, if we write

$$u_{k+1}(z) = \gamma_0 + \gamma_1 z + \gamma_2 z^2 \cdots,$$

$$\mathbf{V}_{k+1}(z) = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1 z + \boldsymbol{\beta}_2 z^2 \cdots$$

and

 $\boldsymbol{\pi}_{k}(z) = \boldsymbol{\alpha}_{0} + \boldsymbol{\alpha}_{1}z + \boldsymbol{\alpha}_{2}z^{2}\cdots + \boldsymbol{\alpha}_{\nu_{k}}z^{\nu_{k}},$ where $\boldsymbol{\alpha}_i, \boldsymbol{\beta}_i \in \mathbb{R}^n$ and $\gamma_i \in \mathbb{R}$ for $i := 0, 1, \cdots$, then we obtain

$$(\gamma_0 + \gamma_1 z + \gamma_2 z^2 \cdots)(\boldsymbol{\alpha}_0 + \boldsymbol{\alpha}_1 z + \boldsymbol{\alpha}_2 z^2 \cdots + \boldsymbol{\alpha}_{\nu_k} z^{\nu_k}) = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1 z + \boldsymbol{\beta}_2 z^2 \cdots + O(z^{\nu_k+1})$$

since by construction, $S_{k+1}(0)$, and so γ_0 and β_0 , do not vanish. By comparing coefficients of powers of z, we may derive a triangular set of equations for the coefficients of $\pi_k(z)$, which may be solved by forward substitution to yield

$$\boldsymbol{\alpha}_0 = \frac{\boldsymbol{\beta}_0}{\gamma_0} \quad \alpha_i = \frac{1}{\gamma_0} [\boldsymbol{\beta}_i - \sum_{j=0}^{i-1} \boldsymbol{\alpha}_j \gamma_{i-j}] \quad i := 1, 2 \cdots, \nu_k$$

The initializations become

$$\begin{aligned}
 \mathbf{V}_{1}(z) &:= \mathbf{f}(z) & \text{and} & u_{0}(z) := \mathbf{f}(z) \cdot \mathbf{f}(z) &, & u_{1}(z) := 1 \\
 \pi_{0} &:= \mathbf{f}(0) & \nu_{0} := 0 \\
 \mu_{1} &:= O[\mathbf{V}_{1}(z) - \boldsymbol{\pi}_{0}(z)u_{1}(z)] & \nu_{1} := \mu_{1}
 \end{aligned}$$
(4.7)

Graves-Morris *et al.* (1994) show that the successive convergents of (4.1), $\mathbf{C}_k(z)$, are the $[\tau_k/\tau_k]$ vector Padé approximants of $\mathbf{f}(z)$ (correspondence), where $\tau_k := \sum_{i=0}^k \nu_i$. In fact, the following order condition is satisfied $(\nu_{k+1} \ge 1)$:

$$\mathbf{f}(z) - \mathbf{C}_k(z) = O(z^{2\tau_k + \nu_{k+1}}).$$

In the case of non-degeneracy we have $\tau_k = k$ since

$$\nu_0 = 0$$
, $\nu_1 = \mu_1 = 1$, $\nu_k = 1$, $\mu_k = 2$ for $k \ge 2$

so that

$$\mathbf{f}(z) = \boldsymbol{\pi}_0 + z [\boldsymbol{\pi}_1(z) + z^2 [\boldsymbol{\pi}_2(z) + z^2 [\boldsymbol{\pi}_3(z) \cdots]^{-1}]^{-1}]^{-1}$$

where each $\pi_k(z), k := 1, 2 \cdots$ is a linear polynomial with real vector coefficients. Hence, in this case, the [m/m] diagonal approximant is given, not by the $2m^{th}$ convergent as in Viskovatov's approach, but by $\mathbf{C}_m(z)$, which requires fewer applications of the recurrence relations.

In the general case, each of the diagonal approximants may be constructed using either backward recurrence relations or a forward version similar to (3.16) Indeed, we point out that, in the spirit of this paper, it is possible to render these relations into a form which does not involve general Clifford elements, but only vectors and scalars — Roberts (1992).

The [l/m] VPA for l > m, if it exists, is given by :

$$p^{[l/m]}(z)[q^{[l/m]}(z)]^{-1} = \mathbf{c}_0 + \mathbf{c}_1 z + \dots + z^{l-m-1} \mathbf{c}_{l-m-1} + z^{l-m} [m/m]_{\mathbf{h}}(z)$$
(4.8)

in which $[m/m]_{\mathbf{h}}(z)$ is the diagonal approximant to

$$\mathbf{h}(z) := \mathbf{c}_{l-m} + \mathbf{c}_{l-m+1}z + \dots + z^{2m}\mathbf{c}_{l+m} + \dots$$
(4.9)

constructed using the above algorithm (for an appropriate value of k). Use of forward recurrence relations implies that $q^{[l/m]}(0) = \pi_1(0)\pi_2(0)\cdots\pi_k(0) \in \Gamma_n$. We point out that only the first 2m + 1 coefficients of $\mathbf{h}(z)$ are required — i.e. those actually quoted above. We shall require the following result (Roberts 1990) :

$$[l/m](z) = \mathbf{P}^{l+m}(z)/Q_{2m}(z).$$
(4.10)

where $Q_{2m}(z)$ is a real analytic polynomial of even degree 2m given by

$$q^{[l/m]}(z)q^{\widetilde{[l/m]}}(z) = Q_{2m}(z)\mathbf{e}_0 \in \mathbb{C}.$$
 (4.11)

and each component of $\mathbf{P}^{l+m}(z)$ is a real analytic polynomial of maximum degree (l+m) defined by

$$p^{[l/m]}(z)q^{\widetilde{[l/m]}}(z) = \sum_{i=1}^{n} P_i^{l+m}(z)\mathbf{e}_i \in \mathbb{C}^n.$$
(4.12)

In order to construct approximants [l/m] where l < m we consider the inverse series for $\mathbf{f}(z)$, if necessary after extracting an appropriate power of z. The numerators and denominators satisfy similar properties to those outlined above.

5 An Application — New Approximants

In this section, after introducing an application of vector Padé approximants, which echoes the origins of this subject in the work of Wynn, we focus on an apparent disadvantage of these constructs in this context, and then develop a modified form, based on their Clifford algebraic description, which may produce a better performance. The motivation for this procedure is founded on both theoretical reasons and results of numerical experiments.

Suppose we are given a sequence of real vectors $\{\mathbf{s}_l\}$ $l := 0, 1, \cdots$, which converges slowly to some limit \mathbf{s} . The convergence of this sequence is accelerated if we can construct a new sequence $\{\mathbf{t}_l\}$ which converges faster to \mathbf{s} . One approach is to consider the generating function given (perhaps formally) by the power series (2.1), in which $\mathbf{c}_0 := \mathbf{s}_0$, $\mathbf{c}_l := \Delta \mathbf{s}_{l-1} := \mathbf{s}_l - \mathbf{s}_{l-1}$, for $l = 1, 2, \cdots$, such that $\mathbf{f}(1) = \mathbf{s}$. Our task then becomes one of approximating $\mathbf{f}(z)$ at z = 1. This may be attempted using vector Padé approximants — e.g. $\mathbf{t}_l := [l/m](1)$ for fixed m - c.f.Roberts 1995. If the sequence $\{\mathbf{s}_l\}$ is generated from a matrix iterative method of solving a system of linear equations then $\mathbf{f}(z)$ belongs to a certain class of functions characterised as follows (Graves-Morris 1992):

$$\mathbf{f}(z) := \frac{\mathbf{g}(z)}{\lambda(z)} \tag{5.1}$$

where $\lambda(z)$ is the monic polynomial $\prod_{i=1}^{m}(z - \alpha_i)$ in which the complex numbers α_i , $i = 1, \ldots, m$, satisfy $0 < |\alpha_i| < \rho$. The $g_j(z), j = 1, 2, \ldots, n$, are complexvalued functions analytic in $D_{\rho} := \{z : |z| < \rho\}$. The Maclaurin series for $\mathbf{f}(z)$ may be determined and is of the form (2.1) if $\lambda(z)$ and each $g_j(z), j := 1, \cdots, n$ are real analytic functions. Our concern is with the formation of [l/m] approximants to $\mathbf{f}(z)$ for increasing values of l. Roberts (1994) proves a theorem governing the convergence of approximants along this row of the vector Padé table assuming that

$$\mathbf{g}(\alpha_i) \cdot \mathbf{g}(\alpha_i) \neq 0, \quad i = 1, 2, \dots, m.$$
(5.2)

In this paper we are particularly interested in the result that, as $l \to \infty$, the monic denominators $q^{[l/m]}(z)$ converge uniformly to $\lambda(z)\mathbf{e}_0$ in compact subsets of the complex plane. We also note that the numerators $p^{[l/m]}(z)$ converge uniformly to $\mathbf{g}(z)$ in compact subsets of D_{ρ} . The norm used is the absolute or spinor norm on $\mathcal{C}\ell(\mathbb{C}^n)$ — see e.g. Hile and Lounesto.

The vector ϵ -algorithm may be employed, as suggested by Wynn in 1962, to construct the desired approximant at z = 1. However, from (4.10) we observe that each [l/m] VPA has, in general, 2m poles — twice as many as required! It is only in the limit of l tending to infinity that cancellation with numerator factors is guaranteed, thus leaving the correct number of poles. Graves-Morris (1994a,b)

suggested that this doubling of poles leads to poor approximations of $\mathbf{f}(z)$, which in turn yields disappointing acceleration results.

The monic denominator may be written as

$$q^{[l/m]}(z) := q_0^{[l/m]}(z)\mathbf{e}_0 + \sum_{J \neq \emptyset} q_J^{[l/m]}(z)\mathbf{e}_J$$
(5.3)

where J denotes the multi-ordered index $\{j_1, j_2, \dots, j_k\}$ in which $1 \leq j_1 < j_2 < \cdots < j_k \leq n$ and each \mathbf{e}_J represents the basis element $\mathbf{e}_{j_1} \mathbf{e}_{j_2} \cdots \mathbf{e}_{j_k}$ of $C\ell_n$; $q_0^{[l/m]}(z)$ is a scalar monic polynomial of exact degree m, while each $q_J^{[l/m]}(z), J \neq \emptyset$, is a scalar polynomial of degree strictly less than m. Then $q_0^{[l/m]}(z)$ is at least as good an approximation to $\lambda(z)$ as the full [Clifford VPA] polynomial $q^{[l/m]}(z)$ in the sense that

$$|q_0^{[l/m]}(z) - \lambda(z)| \le |q^{[l/m]}(z) - \lambda(z)\mathbf{e}_0|$$
(5.4)

since

$$|q^{[l/m]}(z) - \lambda(z)\mathbf{e}_0|^2 := |q_0^{[l/m]}(z) - \lambda(z)|^2 + \sum_{J \neq \emptyset} |q_J^{[l/m]}(z)|^2.$$
(5.5)

A numerator polynomial may be constructed by imposing the order condition (2.3):

$$\mathbf{p}^{(l,m)}(z) := [\mathbf{f}(z)q^{(l,m)}(z)]_0^{l+m}$$
(5.6)

where the new denominator is denoted by $q^{(l,m)}(z)$. An alternative definition would be to retain the numerator degree (i.e. l), thus reducing the order of approximation to $\mathbf{f}(z)$.

Furthermore, if the $g_j(z)$ for $j := 1, 2 \cdots, n$, are in fact polynomials of maximum degree l then, from the uniqueness property of VPA's, we obtain

$$[l/m](z) \equiv \mathbf{f}(z)$$

leading to

$$\begin{split} q_0^{[l/m]}(z) &\equiv \lambda(z) \ , \quad q_J^{[l/m]}(z) \equiv 0 \ J \neq \emptyset \\ \text{and} \ p^{[l/m]}(z) &\equiv \mathbf{g}(z) \end{split}$$

i.e. the new denominator is also exact, as is the corresponding numerator (whichever definition is chosen)

$$\mathbf{p}^{(l,m)}(z) \equiv \mathbf{g}(z).$$

Example 3. We obtain the monic form of the $\lfloor l/1 \rfloor$ denominator from (2.7) viz

$$q^{[l/1]}(z) := z - \mathbf{c}_{l+1}^{-1} \mathbf{c}_l \tag{5.7}$$

which yields

$$q_0^{[l/1]}(z) := z - \frac{\mathbf{c}_{l+1} \cdot \mathbf{c}_l}{\mathbf{c}_{l+1} \cdot \mathbf{c}_{l+1}}$$
(5.8)

using

$$\langle \mathbf{c}_l \mathbf{c}_{l+1} \rangle_0 = \mathbf{c}_l \cdot \mathbf{c}_{l+1}.$$

In order to illustrate the mechanisms at work we consider, in some detail, the [l/1] approximant to a simple generating function, viz

$$\mathbf{f}(z) := \sum_{i=1}^{n} \frac{\gamma_i \mathbf{v}_i}{z - \alpha_i} + \mathbf{v}_0 \tag{5.9}$$

where $\mathbf{v}_j \in \mathbb{R}^n$ for $j = 0, 1, \dots, n$ and $\alpha_i, \gamma_i \in \mathbb{R}$ for $i = 1, \dots, n$. This is the type of function which arises from a matrix iteration : $\mathbf{s}_{l+1} := G\mathbf{s}_l + \mathbf{a}$ with $\mathbf{a}, \mathbf{s}_l \in \mathbb{R}^n$ for $l = 0, 1 \cdots$ and $G \in \mathbb{R}^n \times \mathbb{R}^n$. Each \mathbf{v}_i $(i = 1, \dots, n)$ is a unit eigenvector of G corresponding to the eigenvalue α_i^{-1} . We further assume that there is one dominant pole, α_1 , and that the α_i $(i = 1, \dots, n)$ are distinct quantities satisfying the inequalities

$$0 < |\alpha_1| < |\alpha_2| < |\alpha_3| \le |\alpha_4| \le \cdots \le |\alpha_n|.$$

From the Maclaurin coefficients , $\mathbf{c}_l = -\sum_{i=1}^n \gamma_i \alpha_i^{-l-1} \mathbf{v}_i \ (l > 0)$, we obtain

$$\mathbf{c}_{l+1}^{-1}\mathbf{c}_{l} = \alpha_{1} + \kappa \left[\frac{\alpha_{1}}{\alpha_{2}}\right]^{l+2} \mathbf{a}_{l}^{-1}\mathbf{b}_{l}$$

where

$$\kappa := \frac{\gamma_2}{\gamma_1} (\alpha_2 - \alpha_1)$$
$$\mathbf{a}_l := \mathbf{v}_1 + \sum_{i=2}^n \frac{\gamma_i}{\gamma_1} \left[\frac{\alpha_1}{\alpha_i}\right]^{l+2} \mathbf{v}_i$$
$$\mathbf{b}_l := \mathbf{v}_2 + \sum_{i=3}^n \frac{\gamma_i}{\gamma_2} \left(\frac{\alpha_i - \alpha_1}{\alpha_2 - \alpha_1}\right) \left[\frac{\alpha_2}{\alpha_i}\right]^{l+2} \mathbf{v}_i$$

so that $\mathbf{a}_l \to \mathbf{v}_1$ and $\mathbf{b}_l \to \mathbf{v}_2$ as $l \to \infty$. The above theorem is applicable provided γ_1 is non-zero, since $\mathbf{g}(\alpha_1) = \gamma_1 \mathbf{v}_1$. This requires the initial guess, \mathbf{s}_0 , to contain a component in the \mathbf{v}_1 direction.

If we denote the errors in the denominators of the vector Padé approximant (5.7) and of the new approximant (5.8) by E_V^l and E_N^l respectively, then we may show that

$$E_V^l = \frac{\gamma_2}{\gamma_1} (\alpha_2 - \alpha_1) \left[\frac{\alpha_1}{\alpha_2} \right]^{l+2} + O(\beta^l)$$
(5.10)

and

$$E_N^l = \frac{\gamma_2}{\gamma_1} (\alpha_2 - \alpha_1) \left[\frac{\alpha_1}{\alpha_2} \right]^{l+2} \cos\theta_l + O(\beta^l)$$
(5.11)

where $\beta := \max(|\alpha_1/\alpha_2|^2, |\alpha_1/\alpha_3|)$ and θ_l denotes the angle between \mathbf{a}_l and \mathbf{b}_l . If $\mathbf{v}_1 \cdot \mathbf{v}_2 = \cos\phi \neq 0$ then $\theta_l = \phi + O(\gamma^l)$ where $\gamma := \max(|\alpha_1/\alpha_2|, |\alpha_2/\alpha_3|)$. E_V^l and

 E_N^l are each of order $O(|\alpha_1/\alpha_2|^l)$, with $|E_V^l| > |E_N^l|$, for sufficiently large l, unless $\phi = 0$ in which case $\mathbf{v}_1 = \pm \mathbf{v}_2$, contradicting our assumption of a single dominant eigenvalue.

However, if the vectors \mathbf{v}_i $(i = 1, \dots, n)$ form an *orthonormal system*, then we obtain

$$\theta_l = \frac{\pi}{2} - \frac{\gamma_2}{\gamma_1} \left[\frac{\alpha_1}{\alpha_2} \right]^{l+2} \left[1 + O(\gamma^{2l}) \right]$$
(5.12)

which implies that (5.11) is replaced by

$$E_N^l = \left(\frac{\gamma_2}{\gamma_1}\right)^2 (\alpha_2 - \alpha_1) \left[\frac{\alpha_1}{\alpha_2}\right]^{2l+4} [1 + O(\gamma^{2l})].$$
(5.13)

(In fact, we only require that the system $\{\mathbf{v}_i ; i = 1, \dots, \nu - 1\}$ is orthonormal, with $\mathbf{v}_1 \cdot \mathbf{v}_\nu \neq 0$ provided that $|\alpha_1/\alpha_2|^2 > |\alpha_1/\alpha_\nu|$.) Hence,

$$\lim_{l \to \infty} \frac{(E_V^l)^2}{E_N^l} = \alpha_2 - \alpha_1,$$
 (5.14)

i.e. for large enough l, the new denominator is much more accurate than the original.

Not surprisingly, the above behaviour is reflected in the description of the dominant singularity. The poles of the [l/1] vector Padé approximant are the zeroes of

$$q^{[l/1]}(z)\overline{q^{[l/1]}}(z) \propto (\mathbf{a}_l \cdot \mathbf{a}_l)(z - \alpha_1)^2 - 2(\mathbf{a}_l \cdot \mathbf{b}_l)(z - \alpha_1) + (\mathbf{b}_l \cdot \mathbf{b}_l)$$

(c.f. (4.12)) which are given by z_V and z_V^* where $z_V := \alpha_1 + \epsilon_V^l$ with

$$\epsilon_V^l := \kappa \left[\frac{\alpha_1}{\alpha_2}\right]^{l+2} \frac{|\mathbf{b}_l|}{|\mathbf{a}_l|} e^{i\theta_l}.$$

The zero of $q_0^{[l/1]}(z)$ is

$$z_N := \mathbf{c}_{l+1}^{-1} \cdot \mathbf{c}_l = \alpha_1 + \epsilon_N^l$$

with

$$\epsilon_N^l := \kappa \left[\frac{\alpha_1}{\alpha_2}\right]^{l+2} \frac{|\mathbf{b}_l|}{|\mathbf{a}_l|} \cos\theta_l = \operatorname{Re}(\epsilon_V^l).$$

If $\cos \phi \neq 0$, then the errors $\epsilon_V^l, \epsilon_N^l$ in the pole position are of the same order and

$$\lim_{l \to \infty} \left(\frac{\operatorname{Im}(\epsilon_V^l)}{\operatorname{Re}(\epsilon_V^l)} \right) = \tan\phi.$$

However, in the event of the $\{\mathbf{v}_i\}$ forming an orthonormal system we discover, using (5.12), that

$$\lim_{l \to \infty} \left(\frac{(\operatorname{Im}(\epsilon_V^l))^2}{\operatorname{Re}(\epsilon_V^l)} \right) = \alpha_2 - \alpha_1,$$

i.e. the real part of the VPA pole has twice as many correct significant figures as the imaginary part. Graves-Morris (e.g.1994a) observed this effect in test cases involving infinite-dimensional vectors (functional Padé approximants) in the context of integral equations. The particular problems he considered concerned real symmetric kernels and thus an orthogonal system of characteristic functions, as in the second case above. This led to the construction of a linear denominator whose zero was in fact the real part of the VPA estimate. The ideas presented here have similar consequences, with the advantage that the generalisation beyond the case of a real simple pole is evident, for the results and statements of this section up to equation(5.14) are valid in the case of *complex* vectors and poles. Finally, Graves-Morris (1994a), mentions two related denominators which, in our language, correspond to the scalar part of the denominator polynomials with the monic and Baker normalisations. The asymptotic behaviour of the errors involved is the same in each case.

Employing (5.6), the new numerator is the vector polynomial

$$\mathbf{p}^{(l,1)}(z) = \left(\sum_{i=0}^{l} \mathbf{c}_{i} z^{i}\right) q^{(l,1)}(z) - z^{l+1} \mathbf{c}_{l+1} \frac{[\mathbf{c}_{l+1} \cdot \mathbf{c}_{l}]}{[\mathbf{c}_{l+1} \cdot \mathbf{c}_{l+1}]}$$

leading to the accelerated sequence (z = 1)

$$\mathbf{t}_{l+1} := \mathbf{s}_l - \Delta \mathbf{s}_l \frac{(\Delta \mathbf{s}_{l-1} \cdot \Delta \mathbf{s}_l)}{(\Delta \mathbf{s}_l \cdot \Delta^2 \mathbf{s}_{l-1})}$$

which is a vector generalisation of Aitken's δ^2 method. Da Cunha and Hopkins, using test examples, found that the acceleration can be greatly enhanced using such methods.

Example 4. For m = 2 we have , using (3.16) , and following (4.8) ,

$$q^{[l/2]}(z) = q_4(z) = \pi_1 \pi_2 \pi_3 \pi_4 + z(\pi_3 \pi_4 + \pi_1 \pi_4 + \pi_1 \pi_2) + z^2 \mathbf{e}_0$$

— as an alternative, but equivalent, monic expression to (2.10); hence

$$q_0^{[l/2]}(z) = q^{(l,2)}(z) = z^2 + z(\pi_3 \cdot \pi_4 + \pi_1 \cdot \pi_4 + \pi_1 \cdot \pi_2) + (\pi_1 \cdot \pi_2)(\pi_3 \cdot \pi_4) - (\pi_1 \cdot \pi_3)(\pi_2 \cdot \pi_4) + (\pi_1 \cdot \pi_4)(\pi_2 \cdot \pi_3).$$

It is intriguing to note that, if (2.10) is used — i.e. the Baker normalisation — to compose the new denominator, the result is identical to that presented by Graves-Morris (1994b), using completely different ideas based on Pfaffians.

Returning to the general problem, we present one method of calculating $q_0^{[l/m]}(z)$ based on the corresponding continued fraction to $\mathbf{f}(z)$ introduced earlier. Our approach is illustrated by considering the non-degenerate case using Viskovatov's method. If we define

$$\mathbf{v}_k(z) := [q_{k-1}(z)]^{-1}[q_k(z)] \qquad \qquad k := 1, 2, \cdots \qquad (5.15)$$

then from the forward recurrence relation (3.16), we obtain

$$\mathbf{v}_{k}(z) = \boldsymbol{\pi}_{k} + z[\mathbf{v}_{k-1}(z)]^{-1} \qquad \qquad k := 2, 3, \cdots \qquad (5.16)$$

with $\mathbf{v}_1(z) = \boldsymbol{\pi}_1$. That each of the $\mathbf{v}_k(z)$ is a real (analytic) vector, is readily proved by induction. In order to construct the [l/m] approximant we follow (4.8) and first of all consider the [m/m] approximant to $\mathbf{h}(z)$ (4.9). The corresponding denominator is given by

$$q^{[l/m]}(z) = q_{2m}(z) = \mathbf{v}_1(z)\mathbf{v}_2(z)\cdots\mathbf{v}_{2m}(z).$$
(5.17)

From (3.16) it is readily seen that $q_{2m}(z)$ is monic. A similar expression, involving 2m + 1 vectors, may be derived for the numerator polynomial. We point out that the backward recurrence relations also yield vector products for these polynomials — involving the same sequence of vectors for the numerator as for the denominator, thus saving computation. The scalar part of a product of an even number of vectors is given by

$$\langle \mathbf{v}_1 \mathbf{v}_2 \cdots \mathbf{v}_{2m} \rangle_0 = \frac{1}{m! 2^m} \sum_{\sigma} \epsilon_{\sigma} (\mathbf{v}_{\sigma_1} \cdot \mathbf{v}_{\sigma_2}) (\mathbf{v}_{\sigma_3} \cdot \mathbf{v}_{\sigma_4}) \cdots (\mathbf{v}_{\sigma_{2m-1}} \cdot \mathbf{v}_{\sigma_{2m}})$$

where the summation is over all permutations σ of the integers $1, 2 \cdots, 2m$ and ϵ_{σ} denotes the corresponding parity of the permutation — for example see Miller. The construction of the $\mathbf{v}_k(z)$, given by (5.16), is useful for a numerical calculation of $q^{[l/m]}(z)$ and hence of $q^{(l,m)}(z)$. However, although each $q_k(z)$ is a polynomial over $C\ell_n$, each $\mathbf{v}_k(z)$ is a rational function of z, cancellation of the denominator factors occurring only in the product (5.17). Hence, to determine the new approximant we require algebraic expressions for the polynomials involved. This may be achieved by noting that $w_k(z) := \widetilde{q_k}(z)q_k(z)$ is a real analytic polynomial, while $\mathbf{W}_k(z) := \widetilde{q_{k-1}}(z)q_k(z)$ is a vector of such polynomials. Employing similar arguments to section three, we may derive appropriate recurrence relations from (3.16). It is then straightforward to construct the new approximant.

However, we could adopt an argument similar to that for the denominator — viz by considering the vector part of $p^{[l/m]}(z)$ which will, in fact, form at least as good an approximation to $\mathbf{g}(z)$ as $p^{[l/m]}(z)$ itself. For, from part (iii) of the above theorem, we may conclude that

$$|\langle p^{[l/m]}(z)\rangle_1 - \mathbf{g}(z)| \le |p^{[l/m]}(z) - \mathbf{g}(z)|$$

using the definition of the spinor norm. This may be implemented as a *numerical* computation with z = 1, thus avoiding the need for constructing *polynomials*. We note that if the Modified Euclidean algorithm is used (to reduce the number of iterations) care must be exercised to normalise the denominator properly.

The above ideas serve to illustrate the flexibility and richness of the Clifford algebraic approach in not only forming useful algorithms for the construction of VPA's but also in allowing the invention and analysis of new approximants which have the correct number of singularities and the desired residue behaviour (part (iii) of the theorem). In particular, we have explained how new constructs may yield more accurate results than VPA's. Investigation of the numerical efficacy of the newcomers is currently in progress.

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