

A VECTOR CHEBYSHEV ALGORITHM

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Abstract

We consider polynomials orthogonal relative to a sequence of vectors and derive their recurrence relations within the framework of Clifford algebras. We state sufficient conditions for the existence of a system of such polynomials. The coefficients in the above relations may be computed using a cross-rule which is linked to a vector version of the quotient-difference algorithm, both of which are proved here using designants. An alternative route is to employ a vector variant of the Chebyshev algorithm. This algorithm is established and an implementation presented which does not require general Clifford elements. Finally, we comment on the connection with vector Padé approximants.

Keywords: Clifford algebras, orthogonal polynomials, quotient-difference algorithm, Chebyshev algorithm, vector Padé approximants, designants.

1 Introduction

In the study of rational approximation to power series whose coefficients are *vectors* Clifford algebras provide a useful framework for the derivation of results using methods of proof analogous to those employed in the corresponding scalar theory [7,15].

One particular area of current interest is the search for algorithms to construct these approximants which may be implemented without requiring general elements in the algebra [5,16,17]. For example, a vector version of the quotient-difference algorithm has been developed, which requires *only* vector operations [18]. Once these vectors have been computed we may form recurrence relations by means of which the polynomials connected with an approximant may be determined. If the coefficients

of the power series being considered are the vectors obtained from matrix iteration then the vectors involved in the new algorithm are related to the eigenvectors of the matrix [18].

In the scalar theory of rational approximation the Chebyshev algorithm provides an alternative to the quotient-difference algorithm to calculate the recurrence relation coefficients as well as the polynomials [2,3,4,21]. We propose a vector version of the Chebyshev algorithm which uses only vectors and square matrices of the same dimension in its implementation.

In order to mirror the scalar development, we begin by considering the theory of polynomials orthogonal relative to a sequence of vectors without assuming any results from the theory of vector Padé approximation. The connection with this latter topic is given in section 5. Wynn [22], whose interest was also in vector rational approximation [23], was the first to consider a non-commutative q-d algorithm and related orthogonal polynomials. We derive three-term recurrence relations for these polynomials and at the same time establish the Clifford nature of the coefficients involved. As a by-product, the above-mentioned vector quotient-difference algorithm is proved using designants, which replace determinants in non-commutative algebras.

We are then in a position to discuss the Chebyshev algorithm in a Clifford algebraic setting. After establishing this algorithm we reformulate it in such a way that no general Clifford elements are needed in its implementation.

In the last section we state briefly the link with vector Padé approximants and derive expressions for the first two terms of the error in the $[n - 1/n]$ approximant.

2 Algebraic Preliminaries

The real Clifford algebra of \mathbb{R}^d , \mathcal{Cl}_d , is the associative algebra over \mathbb{R} generated by the orthonormal basis of \mathbb{R}^d , $\{\mathbf{e}_1, \mathbf{e}_2 \cdots \mathbf{e}_d\}$, obeying the anti-commutation relations

$$\mathbf{e}_i \mathbf{e}_j + \mathbf{e}_j \mathbf{e}_i = 2\delta_{i,j} \quad i, j = 1, 2 \cdots, d \quad (2.1)$$

where the algebra identity is 1 [13,14]. We also require the universality property which is guaranteed if $\mathbf{e}_1 \mathbf{e}_2 \cdots \mathbf{e}_d \neq \pm 1$. In this case \mathcal{Cl}_d is a linear space of dimension 2^d spanned by the basis elements

$$\mathbf{e}_I = \mathbf{e}_{i_1 i_2 \cdots i_k} = \mathbf{e}_{i_1} \mathbf{e}_{i_2} \cdots \mathbf{e}_{i_k} \quad (2.2)$$

where $I = \{i_1, i_2, \cdots, i_k\}$ and $1 \leq i_1 < i_2 < \cdots < i_k \leq d$ for $k = 1, 2 \cdots, d$. The identity element corresponds to the empty set. A general element of \mathcal{Cl}_d is given by

$$a = \sum_I a_I \mathbf{e}_I \quad a_I \in \mathbb{R} \quad (2.3)$$

where the summation is over the 2^d different ordered multi-indices I . We shall require the anti-isomorphism of $Cl_d : a \mapsto \tilde{a}$ called *reversion* obtained by reversing the order of factors in \mathbf{e}_I ; hence $\tilde{\tilde{a}} = a$.

We identify each vector $(v_1, v_2, \dots, v_d) \in \mathbb{R}^d$ with an element, $\sum_{i=1}^d v_i \mathbf{e}_i$, of Cl_d , using the common label \mathbf{v} . The anti-commutation relations, (2.1), imply

$$\mathbf{u}\mathbf{v} + \mathbf{v}\mathbf{u} = 2(\mathbf{u} \cdot \mathbf{v}) \quad (2.4)$$

where $\mathbf{u} \cdot \mathbf{v}$ indicates the usual scalar product, $\sum_{i=1}^d u_i v_i$, and

$$\mathbf{u}\mathbf{v}\mathbf{u} = 2(\mathbf{u} \cdot \mathbf{v})\mathbf{u} - (\mathbf{u} \cdot \mathbf{u})\mathbf{v} \in \mathbb{R}^d \quad (2.5)$$

We note that

$$\tilde{\tilde{\mathbf{v}}} = \mathbf{v} \quad (2.6)$$

and

$$\mathbf{v}\mathbf{v} = \mathbf{v} \cdot \mathbf{v}, \quad \mathbf{v} \in \mathbb{R}^d. \quad (2.7)$$

Although Cl_d is not a division algebra for $d > 0$, we observe that non-zero vectors are invertible:

$$\mathbf{v}^{-1} = \frac{\mathbf{v}}{\mathbf{v} \cdot \mathbf{v}}, \quad \mathbf{v} \in \mathbb{R}^d. \quad (2.8)$$

This is identical to the Moore-Penrose generalised inverse of a real vector used in the axiomatic definition of vector rational interpolants, see *e.g.* [6].

In this work we need to consider systems of linear algebraic equations in which the coefficients are elements of Cl_d ; in fact they are vectors. The role of determinants in studying linear systems in a non-commuting algebra may be played by designants, which were invented by Heyting in 1927 and revived more recently by Salam. For an introduction and detailed study of these constructs the reader is referred to these authors [12,19]. We give a brief account of those properties needed for our purposes. Consider the homogeneous system of linear equations :

$$\begin{array}{cccc} a_{11}y_1 & + & a_{12}y_2 & \cdots & a_{1n+1}y_{n+1} & = & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ a_{n1}y_1 & + & a_{n2}y_2 & \cdots & a_{nn+1}y_{n+1} & = & 0 \end{array} \quad (2.9)$$

in which each $a_{ij} \in Cl_d$. The use of designants allows us to eliminate y_1, y_2, \dots, y_{n-1} , in the given order, to obtain

$$B_{n,n}^{(n-1)}y_n + B_{n,n+1}^{(n-1)}y_{n+1} = 0 \quad (2.10)$$

where $B_{p,q}^{(m)}$ is the left designant of order $(m+1)$ with rows $1, 2, \dots, m, p$ and columns $1, 2, \dots, m, q$ with $p, q > m$, [12] p474,

$$B_{p,q}^{(m)} = \begin{vmatrix} a_{11} & \cdots & a_{1m} & a_{1q} \\ \vdots & & \vdots & \vdots \\ a_{m1} & \cdots & a_{mm} & a_{mq} \\ a_{p1} & \cdots & a_{pm} & a_{pq} \end{vmatrix}_l \quad (2.11)$$

In the Appendix we quote an analogue of Sylvester's identity for determinants which may be used to express a designant of order $n + 1$ in terms of designants of order n . The lowest order designant, $B_{1,1}^{(0)}$, is given by a_{11} , thus allowing, in principle, the computation of any designant. Heyting [12] shows that the designant $B_{n,n}^{(n-1)}$ exists if each of the designants $B_{m,m}^{(m-1)}$ exists and is invertible for $m = 1, 2, \dots, n - 1$.

For the inhomogeneous system

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &= b_1 \\ \vdots & \\ a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n &= b_n \end{aligned} \tag{2.12}$$

we may write

$$\begin{aligned} x_n &= y_n [y_{n+1}]^{-1} = -[B_{n,n}^{(n-1)}]^{-1} B_{n,n+1}^{(n-1)} \\ &= \begin{vmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{vmatrix}_l^{-1} \begin{vmatrix} a_{11} & \dots & a_{1n-1} & b_1 \\ \vdots & & \vdots & \vdots \\ a_{n1} & \dots & a_{nn-1} & b_n \end{vmatrix}_l \end{aligned} \tag{2.13}$$

Hence, the above expression for x_n is valid if $B_{m,m}^{(m-1)}$ is invertible for $m = 1, 2, \dots, n$.

Finally, we point out some properties of designants corresponding to those of the matrices of coefficients. If we represent the left designant $B_{n,n}^{(n-1)}$ by $|A|_l$ where A is the array $[a_{ij}]$, then from the nature of equations (2.9) we obtain

$$|\widetilde{A}|_l = |\widetilde{A}|_r = |A|_r = |A^t|_l \tag{2.14}$$

if $\widetilde{A} = A$, using $|A|_r = |A^t|_l$ [12,19], where the superscript t denotes the transpose. Hence, if $A^t = A$ then

$$|\widetilde{A}|_l = |A|_l. \tag{2.15}$$

3 Polynomials orthogonal relative to a vector sequence

We follow and adapt Wall [21] in constructing a sequence of monic polynomials $\{B_n^J(u), n = 0, 1, \dots\}$ orthogonal relative to a given sequence of vectors $\{\mathbf{c}_n \in \mathbb{R}^d, n = J, J + 1, \dots\}$. Instead of using the formal integral approach of Wall we use the bilinear functional

$$\mathbf{c}^{(J)} : Cl_d[u] \times Cl_d[u] \mapsto Cl_d \tag{3.1}$$

defined by

$$\mathbf{c}^{(J)}[bu^m, au^n] := bc_{J+m+n}a \quad \text{for } a, b \in Cl_d \tag{3.2}$$

and extended to all pairs of polynomials over $\mathcal{C}\ell_d$ by linearity in each of the two variables. An alternative is to use left and right functionals — *i.e.* the pre- and post- processes of Wynn [21,22]; see Salam [20] in this context.

The condition of orthogonality relative to the vector sequence $\{\mathbf{c}_J, \mathbf{c}_{J+1}, \mathbf{c}_{J+2} \cdots\}$ is given by

$$\mathbf{c}^{(J)}[B_m^J(u), B_n^J(u)] = 0 \quad \text{for } m \neq n \quad (3.3)$$

which implies

$$\mathbf{c}^{(J)}[u^m, B_n^J(u)] = 0 \quad \text{for } m = 0, 1, \dots, n-1. \quad (3.4)$$

It follows from the definition of $\mathbf{c}^{(J)}$ that

$$\mathbf{c}^{(J)}[\lambda p(u), q(u)\mu] = \lambda \mathbf{c}^{(J)}[p(u), q(u)]\mu \quad (3.5)$$

where $\lambda, \mu \in \mathcal{C}\ell_d$ and $p(u), q(u) \in \mathcal{C}\ell_d[u]$. If we describe $B_n^J(u)$ as follows:

$$B_n^J(u) = u^n + b_{n-1}^{(n,J)}u^{n-1} + b_{n-2}^{(n,J)}u^{n-2} + \cdots + b_1^{(n,J)}u + b_0^{(n,J)} \quad (3.6)$$

in which the coefficients belong to $\mathcal{C}\ell_d$, then the conditions (3.4) lead to the system of linear equations

$$\left. \begin{array}{cccc} \mathbf{c}_J b_0^{(n,J)} & + \mathbf{c}_{J+1} b_1^{(n,J)} & + \cdots & \mathbf{c}_{J+n-1} b_{n-1}^{(n,J)} & = & -\mathbf{c}_{J+n} \\ \mathbf{c}_{J+1} b_0^{(n,J)} & + \mathbf{c}_{J+2} b_1^{(n,J)} & + \cdots & \mathbf{c}_{J+n} b_{n-1}^{(n,J)} & = & -\mathbf{c}_{J+n+1} \\ \vdots & \vdots & & \vdots & \vdots & \\ \mathbf{c}_{J+n-1} b_0^{(n,J)} & + \mathbf{c}_{J+n} b_1^{(n,J)} & + \cdots & \mathbf{c}_{J+2n-2} b_{n-1}^{(n,J)} & = & -\mathbf{c}_{J+2n-1} \end{array} \right\} \quad (3.7)$$

We shall find it convenient to introduce two Clifford elements as follows:

$$\mathbf{U}_n^J := \mathbf{c}^{(J)}[u^n, B_n^J(u)] \quad (3.8)$$

i.e.

$$\mathbf{c}_{J+n} b_0^{(n,J)} + \mathbf{c}_{J+n+1} b_1^{(n,J)} + \cdots + \mathbf{c}_{J+2n-1} b_{n-1}^{(n,J)} - \mathbf{U}_n^J = -\mathbf{c}_{J+2n} \quad (3.9)$$

and

$$T_n^J := \mathbf{c}^{(J)}[u^{n+1}, B_n^J(u)] \quad (3.10)$$

i.e.

$$\mathbf{c}_{J+n+1} b_0^{(n,J)} + \mathbf{c}_{J+n+2} b_1^{(n,J)} + \cdots + \mathbf{c}_{J+2n} b_{n-1}^{(n,J)} - T_n^J = -\mathbf{c}_{J+2n+1} \quad (3.11)$$

Theorem 3.1 below justifies the vector notation for \mathbf{U}_n^J . From (2.13) above and (6.2) in the Appendix it may be seen that \mathbf{U}_n^J is given by a designant reminiscent of a Hankel determinant – see *e.g.* [10].

$$\mathbf{U}_n^J = \begin{vmatrix} \mathbf{c}_J & \mathbf{c}_{J+1} & \cdots & \mathbf{c}_{J+n-1} & \mathbf{c}_{J+n} \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ \mathbf{c}_{J+n-1} & \mathbf{c}_{J+n} & \cdots & \mathbf{c}_{J+2n-2} & \mathbf{c}_{J+2n-1} \\ \mathbf{c}_{J+n} & \mathbf{c}_{J+n+1} & \cdots & \mathbf{c}_{J+2n-1} & \mathbf{c}_{J+2n} \end{vmatrix}_l \quad (3.12)$$

and, since this array is symmetric, (2.15) implies that

$$\widetilde{\mathbf{U}}_n^J = \mathbf{U}_n^J. \quad (3.13)$$

The following theorem constitutes the main result of this section.

Theorem 3.1 *The Clifford elements \mathbf{U}_n^J are vectors in \mathbb{R}^d and satisfy the five-point cross-rule*

$$\mathbf{U}_{n+1}^J = \mathbf{U}_n^{J+2} + \mathbf{U}_n^{J+1}[(\mathbf{U}_{n-1}^{J+2})^{-1} - (\mathbf{U}_n^J)^{-1}]\mathbf{U}_n^{J+1} \quad (3.14)$$

with the initialisations

$$\mathbf{U}_{-1}^J := \infty, \quad J = 2, 3, \dots \quad \text{and} \quad \mathbf{U}_0^J := \mathbf{c}_J, \quad J = 0, 1, 2, \dots \quad (3.15)$$

Proof From the system composed of (3.7) and (3.11) T_n^J is given by

$$T_n^J = \begin{vmatrix} \mathbf{c}_J & \mathbf{c}_{J+1} & \cdots & \mathbf{c}_{J+n-1} & \mathbf{c}_{J+n} \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ \mathbf{c}_{J+n-1} & \mathbf{c}_{J+n} & \cdots & \mathbf{c}_{J+2n-2} & \mathbf{c}_{J+2n-1} \\ \mathbf{c}_{J+n+1} & \mathbf{c}_{J+n+2} & \cdots & \mathbf{c}_{J+2n} & \mathbf{c}_{J+2n+1} \end{vmatrix}_l \quad (3.16)$$

using (2.13) and (6.2).

Schwein's identity (6.3) applied to $[\mathbf{U}_n^J]^{-1}\widetilde{T}_n^J$ yields

$$[\mathbf{U}_n^J]^{-1}\widetilde{T}_n^J = [\mathbf{U}_{n-1}^{J+1}]^{-1}\widetilde{T}_{n-1}^{J+1} + [\mathbf{U}_n^J]^{-1}\mathbf{U}_n^{J+1}.$$

Hence, if

$$W_n^J := -[\mathbf{U}_n^J]^{-1}\widetilde{T}_n^J \quad (3.17)$$

then

$$W_{n-1}^{J+1} - W_n^J = [\mathbf{U}_n^J]^{-1}\mathbf{U}_n^{J+1} =: q_{n+1}^J \quad (3.18)$$

anticipating a link established later in this paper.

Applying the analogue of Sylvester's identity (6.1) to \mathbf{U}_{n+1}^J , we obtain

$$\mathbf{U}_{n+1}^J = X_n^J - T_n^J[\mathbf{U}_n^J]^{-1}\widetilde{T}_n^J \quad (3.19)$$

in which

$$X_n^J := \begin{vmatrix} \mathbf{c}_J & \mathbf{c}_{J+1} & \cdots & \mathbf{c}_{J+n-1} & \mathbf{c}_{J+n+1} \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ \mathbf{c}_{J+n-1} & \mathbf{c}_{J+n} & \cdots & \mathbf{c}_{J+2n-2} & \mathbf{c}_{J+2n} \\ \mathbf{c}_{J+n+1} & \mathbf{c}_{J+n+2} & \cdots & \mathbf{c}_{J+2n} & \mathbf{c}_{J+2n+2} \end{vmatrix}_l \quad (3.20)$$

Applying Schwein's identity (6.3) to $[T_n^J]^{-1}X_n^J$ yields

$$[T_n^J]^{-1}X_n^J = [\mathbf{U}_{n-1}^{J+1}]^{-1}\widetilde{T}_{n-1}^{J+1} + [T_n^J]^{-1}T_n^{J+1}. \quad (3.21)$$

If T_n^J is not invertible then the relationship (3.21) should be rephrased by multiplying on the left by T_n^J . We remind the reader that any non-zero vector in \mathbb{R}^d is invertible.

Eliminating X_n^J from (3.19) and (3.21) produces

$$\mathbf{U}_{n+1}^J = T_n^{J+1} + T_n^J \{ [\mathbf{U}_{n-1}^{J+1}]^{-1} \widetilde{T}_{n-1}^{J+1} - [\mathbf{U}_n^J]^{-1} \widetilde{T}_n^J \} \quad (3.22)$$

which, with (3.17),(3.18),(3.13) and reversion, finally yields

$$W_n^J - W_n^{J+1} = [\mathbf{U}_n^{J+1}]^{-1} \mathbf{U}_{n+1}^J =: e_{n+1}^J \quad (3.23)$$

Using equations (3.18) and (3.23) to express the nominated quantities in terms of differences in W elements, we observe that

$$e_{n+1}^J + q_{n+1}^J = e_n^{J+1} + q_{n+1}^{J+1}. \quad (3.24)$$

Fig.1 illustrates the relationships between the Clifford elements q_n^J, e_n^J and W_n^J using definitions (3.18) and (3.23). Each element is the difference of the connected W -elements.

$$\begin{array}{ccccc} W_{n-1}^{J+1} & - & q_{n+1}^J & - & W_n^J \\ | & & & & | \\ e_n^{J+1} & & & & e_{n+1}^J \\ | & & & & | \\ W_{n-1}^{J+2} & - & q_{n+1}^{J+1} & - & W_n^{J+1} \end{array}$$

Figure 1: Elements related by (3.18) and (3.23)

Again using (3.18) and (3.23), but this time choosing the expressions in terms of the vectors \mathbf{U} , we obtain

$$[\mathbf{U}_n^{J+1}]^{-1} \mathbf{U}_{n+1}^J + [\mathbf{U}_n^J]^{-1} \mathbf{U}_n^{J+1} = [\mathbf{U}_{n-1}^{J+2}]^{-1} \mathbf{U}_n^{J+1} + [\mathbf{U}_n^{J+1}]^{-1} \mathbf{U}_n^{J+2} \quad (3.25)$$

which, after multiplying on the left by \mathbf{U}_n^{J+1} establishes the cross-rule eqn(3.14). It is clear from the solution for \mathbf{U}_n^J in eqn(3.12) that the initialisation $\mathbf{U}_0^J = \mathbf{c}_J$ is valid for non-negative J . The rest of the initialisation follows from the observation that

$$\mathbf{U}_1^J = \begin{vmatrix} \mathbf{c}_J & \mathbf{c}_{J+1} \\ \mathbf{c}_{J+1} & \mathbf{c}_{J+2} \end{vmatrix}_l = \mathbf{c}_{J+2} - \mathbf{c}_{J+1} [\mathbf{c}_J]^{-1} \mathbf{c}_{J+1} \quad J \geq 0 \quad (3.26)$$

may be derived from the cross-rule if we set

$$\mathbf{U}_{-1}^J := \infty$$

(3.9). As far as the vector case is concerned, it is demonstrated in [18] that analogous expressions for q_n^J and e_n^J are valid. These expressions are embodied in equations (3.18) and (3.23), and reduce to the usual Hankel formulae for the scalar theory, using the connection between determinants and designants derived in [12,19].

The q_n^J and e_n^J elements may be arrayed in a table as in the scalar case – see *e.g.* [9]. The connection between neighbouring entries is given by the non-commuting rhombus rules as stated in :

Corollary 3.2 *Vector Quotient-difference algorithm*

$$e_{n+1}^J + q_{n+1}^J = q_{n+1}^{J+1} + e_n^{J+1} \quad (3.24)$$

$$e_{n+1}^J q_{n+2}^J = q_{n+1}^{J+1} e_{n+1}^{J+1} \quad (3.27)$$

for $n = 0, 1, 2, \dots$ and $J = 0, 1, 2, \dots$, with

$$\left. \begin{array}{l} e_0^J = 0 \quad \text{for } J = 1, 2, \dots \\ q_1^J = [\mathbf{c}_J]^{-1} \mathbf{c}_{J+1} \quad \text{for } J = 0, 1, 2, \dots \end{array} \right\} \quad (3.28)$$

as initial conditions.

Proof The result (3.24) has been derived above while (3.27) is simply a consequence of the definitions (3.18) and (3.23). The initialisations of Theorem 3.1 for \mathbf{U}_n^J together with equations (3.18) and (3.23) imply (3.28). \square

4 Vector Chebyshev algorithm

One disadvantage of using the cross-rule (3.14) is that, if we wish to calculate only those vectors corresponding to a particular system of orthogonal polynomials, undesired parts of the \mathbf{U} -table have to be computed. Instead of using this approach to construct the $\{\mathbf{U}_n^J : n = 0, 1, \dots\}$, for constant J , we may resort to a vector variant of Chebyshev's algorithm [2,3,4,21]. We begin by describing this algorithm within the context of Clifford algebras and then show how it may be implemented using vectors *only*.

Theorem 4.1 *Given a sequence of vectors $\{\mathbf{c}_n \in \mathbb{R}^d : n = 0, 1, \dots\}$ such that, for fixed J , the (vectorial) designants $\{\mathbf{U}_n^J : n = 0, 1, \dots, N\}$ defined by (3.12), do not vanish, then there exist unique monic polynomials $\{B_n^J(u), n = 0, 1, \dots, N+1\}$ satisfying*

$$\mathbf{c}^{(J)}[B_m^J(u), B_n^J(u)] = 0 \quad \text{for } m \neq n. \quad (4.1)$$

These vector orthogonal polynomials may be constructed using the three-term recurrence relation

$$B_{n+1}^J(u) = B_n^J(u)[u + b_{n+1}^J] - B_{n-1}^J(u)a_n^J \quad B_{-1}^J(u) := 0, \quad B_0^J(u) := 1 \quad (4.2)$$

where the recurrence coefficients are given by

$$a_n^J = [\mathbf{U}_{n-1}^J]^{-1} \mathbf{U}_n^J \quad (4.3a)$$

and

$$b_{n+1}^J = W_n^J - W_{n-1}^J \quad (4.3b)$$

in which the W_n^J are defined by (3.10) and (3.17) i.e.

$$\widetilde{W}_n^J := -\mathbf{c}[u^{n+1}, B_n^J(u)][\mathbf{U}_n^J]^{-1} \quad (4.4)$$

Proof Given any monic polynomial of degree $n+1$ over Cl_d , we may express it as a linear combination of the monic polynomials $B_m^J(u)$, $m = 0, 1, \dots, n$. In particular, for $B_{n+1}^J(u)$ we write

$$B_{n+1}^J(u) = B_n^J(u)[u + b_{n+1}^J] - B_{n-1}^J(u)a_n^J + \sum_{l=0}^{n-2} B_l^J(u)k_l^J \quad (4.5)$$

in which it is important to note that the monic nature of the orthogonal polynomials on the right-hand side allow the new Clifford coefficients to be calculated, *without requiring any divisions*, in terms of the *given* coefficients of $B_{n+1}^J(u)$, in the order $b_{n+1}^J, a_n^J, k_{n-2}^J, \dots, k_0^J$, by comparing powers of u in descending order. We impose the conditions

$$\mathbf{c}^{(J)}[u^m, B_{n+1}^J(u)] = 0 \quad \text{for } m = 0, 1, \dots, n \quad (4.6)$$

which, using (4.5), become

$$\begin{aligned} \mathbf{c}^{(J)}[u^{m+1}, B_n^J(u)] + \mathbf{c}^{(J)}[u^m, B_n^J(u)]b_{n+1}^J - \mathbf{c}^{(J)}[u^m, B_{n-1}^J(u)]a_n^J + \\ \sum_{l=0}^{n-2} \mathbf{c}^{(J)}[u^m, B_l^J(u)]k_l^J = 0 \end{aligned} \quad (4.7)$$

For $m = 0, 1, \dots, n-2$ we may show by induction that the orthogonality properties of the polynomials $\{B_l^J(u), l = 0, 1, \dots, n-2\}$ imply that

$$k_0^J = k_1^J = \dots = k_{n-2}^J = 0$$

provided \mathbf{U}_m^J , i.e. $\mathbf{c}[u^m, B_m^J(u)]$, $m = 0, 1, \dots, n-2$ are invertible i.e. none of them vanish. For $m = n-1$ we obtain

$$\mathbf{U}_n^J = \mathbf{U}_{n-1}^J a_n^J.$$

Hence, if $\mathbf{U}_{n-1}^J \neq \mathbf{0}$, then

$$a_n^J = [\mathbf{U}_{n-1}^J]^{-1} \mathbf{U}_n^J. \quad (4.8)$$

For $m = n$ eqn(4.7) yields

$$0 = T_n^J + \mathbf{U}_n^J b_{n+1}^J - T_{n-1}^J a_n^J \quad (4.9)$$

We show that there is a vector $\mathbf{V}_{n+1}^J \in \mathbb{R}^d$ such that

$$W_n^J - W_{n-1}^J = [\mathbf{U}_n^J]^{-1} \mathbf{V}_{n+1}^J \quad (4.10)$$

by noting that

$$W_{n-1}^J - W_n^J = e_n^J + q_{n+1}^J = [\mathbf{U}_n^J]^{-1} \{ \mathbf{U}_n^{J+1} + \mathbf{U}_n^J [\mathbf{U}_{n-1}^{J+1}]^{-1} \mathbf{U}_n^J \}. \quad (4.11)$$

using (3.18) and (3.23). Hence,

$$\mathbf{V}_{n+1}^J = -\{ \mathbf{U}_n^{J+1} + \mathbf{U}_n^J [\mathbf{U}_{n-1}^{J+1}]^{-1} \mathbf{U}_n^J \} \in \mathbb{R}^d \quad (4.12)$$

using (2.5).

Employing this result and (3.17), (4.9) then yields

$$\mathbf{U}_n^J b_{n+1}^J [\mathbf{U}_n^J]^{-1} = \widetilde{W}_n^J - \widetilde{W}_{n-1}^J = \mathbf{V}_{n+1}^J [\mathbf{U}_n^J]^{-1} = \widetilde{b}_{n+1}^J.$$

The result (4.3b) then follows. The uniqueness of B_{n+1}^J is a consequence of the general nature of the expansion (4.5) for a monic polynomial of degree $n + 1$. \square

We point out that b_{n+1}^J may be computed using

$$b_{n+1}^J = [\mathbf{U}_n^J]^{-1} \mathbf{V}_{n+1}^J \quad (4.13)$$

provided $\mathbf{U}_{n-1}^{J+1} \neq \mathbf{0}$, where the vector \mathbf{V}_{n+1}^J is given by eqn(4.12).

We also note that from eqns(4.11),(3.18) and (3.23)

$$a_n^J = q_n^J e_n^J \quad (4.14a)$$

and

$$b_{n+1}^J = W_n^J - W_{n-1}^J = -(e_n^J + q_{n+1}^J) \quad (4.14b)$$

corresponding to the usual theory , *e.g.* [10] chapter 12. Furthermore,

$$\mathbf{U}_n^J = a_0^J a_1^J \cdots a_n^J \quad (4.15a)$$

and

$$W_n^J = b_1^J + b_2^J + \cdots + b_{n+1}^J \quad (4.15b)$$

— *c.f.* Wall [21] chapter XI.

However, since implementation of Theorem 4.1 requires Clifford multiplication we seek another approach which does not have this disadvantage.

For ease of exposition, since J remains constant, we drop the superscript and discuss the computation of the monic polynomials corresponding to $J = 0$, denoted by $B_n(u)$, with other quantities labelled similarly. The other systems of orthogonal polynomials may be composed in like manner.

We begin by defining two new polynomials as follows

$$Q_n(u) := \widetilde{B_n}(u)B_n(u) \quad (4.16)$$

which is monic of exact degree $2n$, and, if $\mathbf{U}_{n-1} \neq \mathbf{0}$

$$\mathbf{\Omega}_n(u) := \mathbf{u}_{n-1}\widetilde{B_{n-1}}(u)B_n(u), \quad \mathbf{u}_{n-1} := \frac{\mathbf{U}_{n-1}}{|\mathbf{U}_{n-1}|} \quad (4.17)$$

of exact degree $2n - 1$. We prove below that $Q_n(u) \in \mathbb{R}[u]$ and $\mathbf{\Omega}_n(u) \in \mathbb{R}^d[u]$, and derive recurrence relations for them.

We also require the following definitions

$$\mathbf{v}_{n+1} := \frac{\mathbf{V}_{n+1}}{|\mathbf{U}_n|} \quad \beta_n := \frac{|\mathbf{U}_n|}{|\mathbf{U}_{n-1}|} \quad (4.18)$$

and the antisymmetric matrices A_n , $n \geq 1$, of order d whose $(i, j)^{th}$ entry is

$$[A_n]_{ij} := 2[(\mathbf{u}_{n-1})_i(\mathbf{v}_n)_j - (\mathbf{u}_{n-1})_j(\mathbf{v}_n)_i] \quad (4.19)$$

In the following theorem we assume that $\mathbf{U}_n \neq \mathbf{0}$, $n = 0, 1, \dots$.

Theorem 4.2 *A Vector Chebyshev algorithm.*

$$Q_n(u) \in \mathbb{R}[u] \quad , \quad \mathbf{\Omega}_n(u) \in \mathbb{R}^d[u] \quad , \quad n \geq 0 \quad (4.20)$$

Initialisation:

$$Q_{-1}(u) = 0, \quad Q_0(u) = 1, \quad \mathbf{\Omega}_0(u) = \mathbf{0} \quad (4.21)$$

Iteration: for $n = 0, 1, \dots$

$$\mathbf{U}_n = \mathbf{c}[1, Q_n(u)] \quad (4.22)$$

$$\mathbf{V}_{n+1} = \left[\sum_{k=1}^n A_k \right] \mathbf{U}_n - \mathbf{c}[u, Q_n(u)] \quad (4.23)$$

$$\mathbf{\Omega}_{n+1}(u) = Q_n(u)[u\mathbf{u}_n + \mathbf{v}_{n+1}] + \beta_n \mathbf{\Omega}_n(u) - 2\beta_n \mathbf{u}_n(\mathbf{u}_n \cdot \mathbf{\Omega}_n(u)) \quad (4.24)$$

$$Q_{n+1}(u) = 2\mathbf{\Omega}_{n+1}(u) \cdot [u\mathbf{u}_n + \mathbf{v}_{n+1}] - Q_n(u)[u\mathbf{u}_n + \mathbf{v}_{n+1}]^2 + Q_{n-1}(u)\beta_n^2 \quad (4.25)$$

The summation in (4.23) is understood to vanish if $n = 0$.

Proof We prove (4.24) and (4.25) by induction. For $n = 0, 1 \dots$ we note that

$$b_{n+1} = \mathbf{u}_n \mathbf{v}_{n+1} \quad , \quad a_n = \beta_n \mathbf{u}_{n-1} \mathbf{u}_n \quad (4.26)$$

using (4.3a) and (4.13). From (4.2) we have, for $J = 0$,

$$B_1(u) = u + b_1 = \mathbf{u}_0[u\mathbf{u}_0 + \mathbf{v}_1] \quad (4.27)$$

since \mathbf{u}_0 is a unit vector. Therefore,

$$\mathbf{\Omega}_1(u) = \mathbf{u}_0 \widetilde{B_0}(u) B_1(u) = u\mathbf{u}_0 + \mathbf{v}_1 \quad (4.28)$$

using the initialisation for $B_0(u) = 1$. Similarly,

$$Q_1(u) = \widetilde{B_1}(u) B_1(u) = [u\mathbf{u}_0 + \mathbf{v}_1]^2. \quad (4.29)$$

We make the induction assumption that $Q_m(u) \in \mathbb{R}[u]$, $\mathbf{\Omega}_m(u) \in \mathbb{R}^d[u]$, for $m = 0, 1, \dots, n$. This assumption holds for $m = 1$. It is also true that $Q_0(u)$ is a scalar quantity. For $m = n + 1$, (4.2) and (4.26) yield

$$\mathbf{\Omega}_{n+1}(u) = \mathbf{u}_n \widetilde{B_n}(u) \{B_n(u)[u + \mathbf{u}_n \mathbf{v}_{n+1}] - \beta_n B_{n-1}(u) \mathbf{u}_{n-1} \mathbf{u}_n\}. \quad (4.30)$$

Hence, since $Q_n(u)$ is assumed to be scalar,

$$\mathbf{\Omega}_{n+1}(u) = Q_n(u)[u\mathbf{u}_n + \mathbf{v}_{n+1}] - \beta_n \mathbf{u}_n \widetilde{\mathbf{\Omega}_n}(u) \mathbf{u}_n. \quad (4.31)$$

Eqn(4.24) then follows from (2.5) and (2.6), since $\mathbf{\Omega}_n(u)$ is assumed to be a vector. Turning to $Q_{n+1}(u)$ we may use the recurrence relations for $B_{n+1}(u)$ to write

$$\begin{aligned} Q_{n+1}(u) = Q_n(u)[u\mathbf{u}_n + \mathbf{v}_{n+1}]^2 + \beta_n^2 Q_{n-1}(u) - \\ \beta_n \{ \mathbf{\Omega}'_n(u)[u\mathbf{u}_n + \mathbf{v}_{n+1}] + [u\mathbf{u}_n + \mathbf{v}_{n+1}] \mathbf{\Omega}'_n(u) \} \end{aligned} \quad (4.32)$$

where

$$\mathbf{\Omega}'_n(u) := \mathbf{u}_n \mathbf{\Omega}_n(u) \mathbf{u}_n = 2\mathbf{u}_n(\mathbf{u}_n \cdot \mathbf{\Omega}_n(u)) - \mathbf{\Omega}_n \in \mathbb{R}^d[u] \quad (4.33)$$

using (2.5). From (4.31) we obtain an expression for $\mathbf{\Omega}'_n(u)$, which, together with (2.4) yields the required recurrence relation (4.25).

The induction assumption implies that $\mathbf{\Omega}_{n+1}(u)$ is a vector of polynomials, and that $Q_{n+1}(u)$ is a scalar.

To demonstrate (4.22) and (4.23) we begin by proving

$$Q_n(u) = \widetilde{B_n}(u) B_n(u) = B_n(u) \widetilde{B_n}(u). \quad (4.34)$$

By construction $Q_n(u)$, $n \geq 0$, is monic. Hence, since it is not the zero polynomial we can find $\alpha \in \mathbb{R}$ such that $Q_n(\alpha) \neq 0$. Then, since $Q_n(\alpha) \in \mathbb{R}$, $B_n(\alpha)$ has a left inverse. From *e.g.* Herstein [11] chapter 6, it follows that, since $\mathcal{C}l_d$ is finite-dimensional, $B_n(\alpha)$ is invertible with identical left and right inverses. Hence, (4.34) is true for $u = \alpha$. By an argument based on expanding polynomials about

$u = \alpha$, it may be shown that the (4.34) holds if α is a zero of $Q_n(u)$. In passing we note that in [18] it is demonstrated that, for real u , $B_n(u)$ belongs to the Lipschitz group and therefore may be written as a product of vectors, from which fact (4.34) readily follows. Since $Q_n(u)$ and $B_n(u)$ are monic polynomials, we use (4.34) and (3.5) to obtain

$$\mathbf{c}[1, Q_n(u)] = \mathbf{c}[1, B_n(u)\widetilde{B_n(u)}] = \mathbf{c}[u^n, B_n(u)] = \mathbf{U}_n \quad (4.35)$$

using the orthogonality properties of $B_n(u)$.

To prove (4.23) we first of all note that it is straightforward, using the recurrence relations (4.2), to show by induction that

$$B_n(u) = u^n + u^{n-1}W_{n-1} + \dots \quad (4.36)$$

Therefore, using this result and the orthogonality properties of $B_n(u)$ with (3.10),(3.17), (4.10) and (4.35)

$$\begin{aligned} \mathbf{c}[u, B_n(u)\widetilde{B_n(u)}] &= \mathbf{c}[u^{n+1}, B_n(u)] + \mathbf{c}[u^n, B_n(u)]\widetilde{W_{n-1}} \\ &= [\mathbf{U}_n, \widetilde{W_{n-1}}]_- - \mathbf{V}_{n+1} \end{aligned} \quad (4.37)$$

in which $[a, b]_{\pm} := ab \pm ba$. In the usual theory ($d = 1$) this commutator vanishes leaving $\{-\mathbf{V}_{n+1}\}$, in which case the results (4.22) and (4.23) agree with Theorem 1 of [4] ; *i.e.* using the notation of [4]

$$\pi_{2n} \equiv \mathbf{U}_n \quad \pi_{2n+1} \equiv -\mathbf{V}_{n+1}.$$

We note that the anti-commutation relations (2.1) imply that, for $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathbb{R}^d$,

$$[\mathbf{a}, \mathbf{bc}]_- = 2\{(\mathbf{a} \cdot \mathbf{b})\mathbf{c} - (\mathbf{a} \cdot \mathbf{c})\mathbf{b}\} = A\mathbf{a} \quad (4.38)$$

where A is the anti-symmetric matrix

$$A_{i,j} := 2\{b_i c_j - b_j c_i\}. \quad (4.39)$$

The result (4.23) then follows on observing that each $b_k = \mathbf{u}_{k-1}\mathbf{v}_k$ in (4.15b). \square

5 Vector Padé approximants

The vector orthogonal polynomials B_n^J are linked to the $[J + n - 1/n]$ vector Padé approximants to the power series

$$\mathbf{f}(z) = \sum_{i=0}^{\infty} \mathbf{c}_i z^i \quad \mathbf{c}_i \in \mathbb{R}^d. \quad (5.1)$$

This connection may be established by developing (5.1) as a right continued fraction [18]

$$\sum_{i=0}^{J-1} \mathbf{c}_i z^i + z^J \mathbf{c}_J [1 - z q_1^J [1 - z e_1^J [1 - z q_2^J [1 - z e_2^J [1 - \dots]^{-1}]^{-1}]^{-1}]^{-1} \quad (5.2)$$

whose even convergents are

$$\sum_{i=0}^{J-1} \mathbf{c}_i z^i + z^J a_0^J [1 - z b_1^J - z^2 a_1^J [1 - z b_2^J - z^2 a_2^J [\dots]^{-1}]^{-1}]^{-1} \quad (5.3)$$

where a_n^J and b_n^J are given by equations (4.14a, b). The even convergents $\mathbf{C}_{2n}^J(z) = p_n^{(J)}(z)[q_n^{(J)}(z)]^{-1}$ are the $[J + n - 1/n]$ vector Padé approximants to $\mathbf{f}(z)$. Here, $p_n^{(J)}(z)$ and $q_n^{(J)}(z)$ are polynomials in z over $\mathcal{C}l_d$ of degrees $J + n - 1$ and n respectively, such that the Maclaurin expansion of $\mathbf{C}_{2n}^J(z)$ agrees with the first $J + 2n$ terms of $\mathbf{f}(z)$ and $q_n^{(J)}(0) = 1$, adopting the Baker convention. From the system of equations (3.7) and (4.36) we deduce that

$$q_n^{(J)}(z) \equiv z^n B_n^J\left(\frac{1}{z}\right) = 1 + z W_{n-1}^J + \dots \quad (5.4)$$

We may obtain information on the leading terms of the Padé error. From (3.9) and (3.11), we have

$$\mathbf{f}(z) q_n^{(J)}(z) - p_n^{(J)}(z) = z^{J+2n} [\mathbf{U}_n^J + z T_n^J + O(z^2)]. \quad (5.5)$$

Hence,

$$\mathbf{f}(z) - p_n^{(J)}(z)[q_n^{(J)}(z)]^{-1} = z^{J+2n} [\mathbf{U}_n^J + z(T_n^J + \widetilde{T}_n^J) + O(z^2)]$$

which for the case of $J = 0$ becomes

$$\mathbf{f}(z) - [n - 1/n](z) = z^{2n} [\mathbf{U}_n + z \mathbf{U}'_n + O(z^2)]$$

where

$$\mathbf{U}'_n := -\{2\mathbf{V}_{n+1} + [\sum_{k=1}^n D_k] \mathbf{U}_n\}$$

with the square matrix D_k of order d defined in terms of the skew-symmetric matrix A_k and the unit matrix I by

$$D_k := A_k + 2(\mathbf{u}_{k-1} \cdot \mathbf{v}_k)I.$$

Here, use has been made of the following identity

$$\mathbf{abc} + \mathbf{cba} = [\mathbf{a}, \mathbf{bc}]_- + [\mathbf{b}, \mathbf{c}]_+ \mathbf{a} = \mathbf{Aa} + 2(\mathbf{b} \cdot \mathbf{c})\mathbf{a}$$

established with the help of (2.4) and (4.38).

In the scalar case a power series or its corresponding Padé table is said to be *normal* [1] if, for each and every approximant, the numerator and denominator polynomials are of full nominal degree. If we adopt the same terminology for the vector case then $\mathbf{f}(z)$ is *normal* if $\mathbf{U}_n^J \neq \mathbf{0}$ for $J, n \geq 0$. Since $\mathbf{U}_n^J \in \mathbb{R}^d$, the requirement of *normality* guarantees that these vectors are invertible, thus validating all the operations in this paper.

6 Appendix – Two designant identities

We state two identities for designants whose proofs may be found in [12,19] for (i) and [19] for (ii). These references provide arguments for right-handed designants, but the results quoted for the left-handed version readily follow.

(i) Analogue of Sylvester’s identity.

$$B_{n,n}^{(n-1)} = \begin{vmatrix} B_{n-1,n-1}^{(n-2)} & B_{n-1,n}^{(n-2)} \\ B_{n,n-1}^{(n-2)} & B_{n,n}^{(n-2)} \end{vmatrix} := B_{n,n}^{(n-2)} - B_{n,n-1}^{(n-2)} [B_{n-1,n-1}^{(n-2)}]^{-1} B_{n-1,n}^{(n-2)}$$

i.e.

$$\begin{vmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \end{vmatrix}_l = \begin{vmatrix} a_{11} & \cdots & a_{1n-2} & a_{1n} \\ \vdots & & \vdots & \vdots \\ a_{n-21} & \cdots & a_{n-2n-2} & a_{n-2n} \\ a_{n1} & \cdots & a_{nn-2} & a_{nn} \end{vmatrix}_l - \begin{vmatrix} a_{11} & \cdots & a_{1n-2} & a_{1n-1} \\ \vdots & & \vdots & \vdots \\ a_{n-21} & \cdots & a_{n-2n-2} & a_{n-2n-1} \\ a_{n1} & \cdots & a_{nn-2} & a_{nn-1} \end{vmatrix}_l \begin{vmatrix} a_{11} & \cdots & a_{1n-2} & a_{1n-1} \\ \vdots & & \vdots & \vdots \\ a_{n-21} & \cdots & a_{n-2n-2} & a_{n-2n-1} \\ a_{n-11} & \cdots & a_{n-1n-2} & a_{n-1n-1} \end{vmatrix}_l^{-1} \begin{vmatrix} a_{11} & \cdots & a_{1n-2} & a_{1n} \\ \vdots & & \vdots & \vdots \\ a_{n-21} & \cdots & a_{n-2n-2} & a_{n-2n} \\ a_{n-11} & \cdots & a_{n-1n-2} & a_{n-1n} \end{vmatrix}_l \quad (6.1)$$

We note that

$$\begin{vmatrix} a_{11} & \cdots & a_{1n-1} & 0 \\ \vdots & & \vdots & \vdots \\ a_{n-11} & \cdots & a_{n-1n-1} & 0 \\ a_{n1} & \cdots & a_{nn-1} & 1 \end{vmatrix}_l = \begin{vmatrix} a_{11} & \cdots & a_{1n-2} & 0 \\ \vdots & & \vdots & \vdots \\ a_{n-21} & \cdots & a_{n-2n-2} & 0 \\ a_{n1} & \cdots & a_{nn-2} & 1 \end{vmatrix}_l = \cdots = \begin{vmatrix} a_{11} & 0 \\ a_{21} & 1 \end{vmatrix}_l = 1 \quad (6.2)$$

since the last column of the last designant of (6.1) is always composed of zeroes.

(ii) Analogue of Schwein's identity.

$$\begin{aligned}
& \left| \begin{array}{cccc} a_{11} & \cdots & a_{1n} & g_1 \\ \vdots & & \vdots & \vdots \\ a_{n1} & \cdots & a_{nn} & g_n \\ a_{n+11} & \cdots & a_{n+1n} & g_{n+1} \end{array} \right|_l^{-1} \left| \begin{array}{cccc} a_{11} & \cdots & a_{1n} & h_1 \\ \vdots & & \vdots & \vdots \\ a_{n1} & \cdots & a_{nn} & h_n \\ a_{n+11} & \cdots & a_{n+1n} & h_{n+1} \end{array} \right|_l = \\
& \left| \begin{array}{cccc} a_{12} & \cdots & a_{1n} & g_1 \\ \vdots & & \vdots & \vdots \\ a_{n2} & \cdots & a_{nn} & g_n \end{array} \right|_l^{-1} \left| \begin{array}{cccc} a_{12} & \cdots & a_{1n} & h_1 \\ \vdots & & \vdots & \vdots \\ a_{n2} & \cdots & a_{nn} & h_n \end{array} \right|_l + \tag{6.3} \\
& \left| \begin{array}{cccc} a_{11} & \cdots & a_{1n} & g_1 \\ \vdots & & \vdots & \vdots \\ a_{n1} & \cdots & a_{nn} & g_n \\ a_{n+11} & \cdots & a_{n+1n} & g_{n+1} \end{array} \right|_l^{-1} \left| \begin{array}{cccc} a_{12} & \cdots & a_{1n} & g_1 & h_1 \\ \vdots & & \vdots & \vdots & \vdots \\ a_{n+12} & \cdots & a_{n+1n} & g_{n+1} & h_{n+1} \end{array} \right|_l
\end{aligned}$$

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