On expansions in orthogonal polynomials

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Abstract

A recently introduced fast algorithm for the computation of the first N terms in an expansion of an analytic function into ultraspherical polynomials consists of three steps: Firstly, each expansion coefficient is represented as a linear combination of derivatives; secondly, it is represented, using the Cauchy integral formula, as a contour integral of the function multiplied by a kernel; finally, the integrand is transformed to accelerate the convergence of the Taylor expansion of the kernel, allowing for rapid computation using Fast Fourier Transform. In the current paper we demonstrate that the first two steps remain valid in the general setting of orthogonal polynomials on the real line with finite support, orthogonal polynomials on the unit circle and Laurent orthogonal polynomials on the unit circle.

1 Introduction

Let $\mathrm{d}\mu$ be a Borel measure defined on Γ, a rectifiable Jordan curve in $\mathbb{C}$, and consider the inner product

$$\langle f, g\rangle_\mu = \int_\Gamma f(z)\bar{g}(z)\,\mathrm{d}\mu(z).$$

Functions f bounded in the norm $\|\cdot\|_\mu = \sqrt{\langle\,\cdot\,,\,\cdot\,\rangle_\mu}$ form a separable Hilbert space $\mathrm{L}_\mu(\Gamma)$. Given a dense orthogonal sequence $\{\varphi_n\}_{n\in\mathbb{Z}_+}$ in $\mathrm{L}_\mu(\Gamma)$, it is elementary that for every $f \in \mathrm{L}_\mu(\Gamma)$ the expansion

$$f(z) \sim \sum_{n=0}^{\infty} \hat{f}_n\varphi_n(z), \qquad \text{where} \qquad \hat{f} = \frac{\langle f, \varphi_n\rangle_\mu}{\|\varphi_n\|_\mu^2}, \quad n \in \mathbb{Z}_+, \tag{1.1}$$

converges in norm. Provided that f and φ_n are $\mathrm{C}^\infty[\Gamma]$ and that $\mathrm{d}\mu$ is absolutely continuous, the convergence in (1.1) is both pointwise and *spectral:* as $N \to \infty$, $\left\| f - \sum_{n=0}^N \hat{f}_n \varphi_n \right\|_\mu \le N^{-\alpha}$ for every $\alpha > 0$. In particular, if f and φ_n are analytic in an open neighbourhood of Γ then there exist $c, \beta > 0$ such that $\left\| f - \sum_{n=0}^N \hat{f}_n \varphi_n \right\|_\mu \le c\mathrm{e}^{-\beta N}$ for $N \gg 1$. This extraordinarily fast rate of convergence explains the important role of expansions (1.1) in numerical computations, in particular in spectral methods for differential equations.

Yet, to be of practical use, the expansion (1.1) must fulfil an additional requirement: we should be able to compute rapidly the coefficients $\hat{f}_n$ to requisite accuracy. The quintessential example is the *Fourier expansion,* $\Gamma = \mathbb{T}$, the positively-oriented complex unit circle, $\mu(z) = z$ and $\varphi_{2n}(z) = z^{-n}$, $\varphi_{2n+1}(z) = z^n$, $n \in \mathbb{Z}_+$. In that case the $\hat{f}_n$s for $n = 0, 1, \ldots, N-1$ can be computed to high accuracy in $\mathcal{O}(N \log_2 N)$ operations using the Fast Fourier Transform (FFT).

Since a simple change of variables converts the Chebyshev integral

$$\int_{-1}^{1} f(x)\mathrm{T}_n(x)\frac{\mathrm{d}x}{(1-x^2)^{1/2}}$$

to the Fourier integral

$$\int_{-\pi}^{\pi} f(\cos\theta)\cos n\theta \,\mathrm{d}\theta,$$

FFT can be also used to calculate a Chebyshev expansion (i.e., $\Gamma = (-1,1)$, $\mathrm{d}\mu = \mathrm{d}x/(1-x^2)^{1/2}$) in $\mathcal{O}(N \log_2 N)$ operations: we call such an expansion "fast". This is the oldest example of a fast expansion in orthogonal polynomials.

There has been some interest in the last few decades in fast algorithms for other expansions in orthogonal polynomials. Alpert & Rokhlin (1991) have introduced a method for fast computation of expansions in Legendre polynomials using the fast multipole technique. Unfortunately, their algorithm is very complicated, does not lend itself easily to a multivariate interpretation (which is critical to most applications to spectral methods) and is not in wide use. Potts, Steidl & Tasche (1998) introduced a general methodology, combining Clenshaw–Curtis quadrature and divide-and-conquer techniques, for the computation of expansions in general orthogonal polynomials when Γ is a bounded real interval.

Recently, Iserles (2011) introduced a fast algorithm for the computation of Legendre expansions (that is, $\Gamma = (-1,1)$ and $\mu(x) = x$, whereby $\varphi_n = \mathrm{P}_n$, the standard Legendre polynomial). This has been generalised by Cantero & Iserles (2011) to $\Gamma = (-1,1)$ and $\mathrm{d}\mu(x) = (1-x^2)^\alpha \,\mathrm{d}x$, where $\alpha > -1$. The underlying orthogonal polynomials are the *ultraspherical polynomials* $\varphi_n = \mathrm{P}_n^{(\alpha,\alpha)}$ (known, under different normalisation, as *Gegenbauer polynomials.*) and their special cases include Legendre polynomials and Chebyshev polynomials of first and second kind. This approach rests upon three conceptual (and often counter-intuitive) steps, which we present in a general setting. We assume without loss of generality that $0 \in \Gamma$.

1. Express x^n explicitly as a linear combination of φ_m, $m = 0, 1, \ldots, n$,

$$x^n = \sum_{m=0}^{n} d_{n,m} \varphi_m(x), \qquad n \in \mathbb{Z}_+. \tag{1.2}$$

   This is always possible, because $\{\varphi_0, \varphi_1, \ldots, \varphi_n\}$ form a basis of $\mathbb{P}_n$, the linear space of polynomials of degree less or equal to n.

   Given an analytic function $f(x) = \sum_{n=0}^{\infty} f^{(n)}(0) x^n / n!$, we can thus write it in the form

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \sum_{m=0}^{n} d_{n,m} \varphi_m(x) = \sum_{m=0}^{\infty} \left[\sum_{n=m}^{\infty} d_{n,m} \frac{f^{(n)}(0)}{n!} \right] \varphi_m(x).$$

   Therefore

$$\hat{f}_m = \sum_{n=m}^{\infty} d_{n,m} \frac{f^{(n)}(0)}{n!}, \qquad m \in \mathbb{Z}_+. \tag{1.3}$$

2. Let Γ be bounded and γ be a closed Jordan curve encircling Γ within the domain of analyticity of f with winding number 1. Using the Cauchy Integral Theorem, we express (1.3) in the form

$$\hat{f}_m = \frac{1}{2\pi \mathrm{i}} \int_\gamma f(z) K_m(z) \,\mathrm{d}z, \qquad \text{where} \qquad K_m(z) = \sum_{n=m}^{\infty} \frac{d_{n,m}}{z^{n+1}}. \tag{1.4}$$

3. Although it is often possible to choose a trajectory γ so that (1.4) for $m = 0, 1, \ldots, N-1$ can be computed (once the expansion of K_m is truncated) using FFT, this is not a viable approach, because (at least for ultraspherical polynomials) the expansion of K_m converges exceedingly slowly: we need to take $\mathcal{O}(m)$ terms in the truncation of K_m and the outcome is an $\mathcal{O}(N^2)$ algorithm – not good enough! Fortunately, at least for the ultraspherical case, it is possible to subject K_m to a further transformation, which results in a new integral with a rapidly convergent kernel. Such a transformation, in tandem with a specific choice of the curve γ as a Bernstein ellipse, allows for fast computation of $\hat{f}_m$, $m = 0, 1, \ldots, N-1$, using FFT (Cantero & Iserles 2011).

It is instructive in clarifying our argument to show the different steps in the case of ultraspherical polynomials (Cantero & Iserles 2011). Thus, (1.2) is

$$x^n = \frac{n!}{2^n} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{\alpha + n - 2m + \frac{1}{2}}{m! (\alpha + \frac{1}{2})_{n-m+1}} \cdot \frac{(2\alpha+1)_{n-2m}}{(\alpha+1)_{n-2m}} \mathrm{P}_{n-2m}^{(\alpha,\alpha)}(x),$$

where $(z)_n$ is the *Pochhammer symbol*, $(z)_0 = 1$, $(z)_{n+1} = (z+n)(z)_n$ for $n \in \mathbb{Z}_+$, therefore

$$d_{n,n-2m} = \frac{n!}{2^n} \cdot \frac{\alpha + n - 2m + \frac{1}{2}}{m! (\alpha + \frac{1}{2})_{n-m+1}} \cdot \frac{(2\alpha+1)_{n-2m}}{(\alpha+1)_{n-2m}}, \qquad m = 0, 1, \ldots, \lfloor n/2 \rfloor,$$

while $d_{n,n-2m-1}=0$, $m=0,1,\ldots,\lfloor(n-1)/2\rfloor$. Thus, (1.3) becomes

$$\hat{f}_m=\sum_{k=0}^{\infty}\frac{d_{2k+m,2k-m}}{(2k+m)!}f^{(2k+m)}(0)=\sum_{k=0}^{\infty}\frac{(\alpha+2k-m+\frac{1}{2})(2\alpha+1)_{2k-m}}{2^{m+2k}m!(\alpha+\frac{1}{2})_{2k+1}(\alpha+1)_{2k-m}}f^{(2k+m)}(0),$$

while (1.4) assumes the form

$$K_n(z)=\frac{(2\alpha+1)_n n!}{2^n(\alpha+\frac{1}{2})_n(\alpha+1)_n}{}_2\mathrm{F}_1\left[\begin{array}{l}\frac{n+1}{2},\frac{n+2}{2};\\ \alpha+n+\frac{3}{2};\end{array}\ \frac{1}{z^2}\right],\qquad n\in\mathbb{Z}_+,\tag{1.5}$$

where ${}_2\mathrm{F}_1$ is the familiar *hypergeometric function* (Rainville 1960).

While steps 1 and 2 for ultraspherical polynomials follow a set pattern, the transformation in step 3 is more a matter of magic. Specifically, the kernel K_n, with slowly-convergent Taylor expansion, is transformed by means of the identity

$${}_2\mathrm{F}_1\left[\begin{array}{l}a,a+\frac{1}{2};\\ c;\end{array}\ 2\zeta-\zeta^2\right]=(1-\tfrac{1}{2}\zeta)^{-2a}{}_2\mathrm{F}_1\left[\begin{array}{l}2a,2a-c+1;\\ c;\end{array}\ \frac{\zeta}{2-\zeta}\right]$$

into a fast convergent function. In particular, once γ in step 2 is chosen as a Bernstein ellipse $\{\frac{1}{2}(\rho\mathrm{e}^{\mathrm{i}\theta}+\rho^{-1}\mathrm{e}^{-\mathrm{i}\theta})\,:\,\theta\in[-\pi,\pi]\}$, where $\rho\in(0,1)$, the transformed integral can be computed fast by means of FFT.

The goal of this paper is to explore the methodology of (Cantero & Iserles 2011) in a much more general setting. Clearly, step 1 can be accomplished *in principle* for any set of orthogonal polynomials – indeed, for any basis of the linear space of polynomials. However, in Section 2 we demonstrate that when Γ is real the coefficients $d_{n,m}$ in (1.2) can be derived in an explicit manner using the underlying Jacobi matrix. If, in addition, Γ is bounded, we also find an explicit expression for the kernel K_n in (1.4) in terms of the resolvent of the underlying Jacobi matrix.

While Section 2 is devoted to orthogonal polynomials on the real line (OPRL), in Section 3 we consider orthogonal polynomials on the unit circle (OPUC), $\Gamma=\mathbb{T}$. The importance of OPUC and much of recent interest in this construct is motivated by their applications in random-matrix theory and spectral analysis (Simon 2005). Again, steps 1 and 2 can be accomplished formally in terms of a matrix associated (like the Jacobi matrix in the OPRL case) with a recurrence relation and its resolvent, respectively.

In Section 4 we abandon the algebraic polynomial framework altogether, considering instead sequences of orthogonal Laurent polynomials (i.e., polynomials in z and z^{-1}) on the unit circle $\mathbb{T}$ (SOLP) (Simon 2005). The narrative repeats itself: the representation (1.2) can be accomplished explicitly in terms of the *CMV matrix* (Cantero, Moral & Velázquez 2003), which originates in recurrence relations for normalised SOLP, while the kernel of the Cauchy Theorem formula (1.4) is expressed in terms of the resolvent of the CMV matrix.

Steps 1 and 2 of our ‘grand scheme’ can be thus accomplished for a large variety of orthogonal systems: OPRL, OPUC and SOLP. This leaves out the all-important step 3: a transformation accelerating the convergence of the kernel K_n, thereby enabling fast computation of expansion coefficients. In the case of ultraspherical polynomials, this step is frankly serendipitous: we know that it works, we can *prove* that it works, we can demonstrate that it works by numerical computations – yet, we cannot understand *why* it works. It is to be hoped that the understanding of this process will be gained in future work, thereby turning serendipity into a general technique and allowing for rapid computation of general expansions in orthogonal polynomials or Laurent polynomials. The main purpose of this paper is to set the stage for this eventuality.

2 Orthogonal polynomials on the real line

2.1 Expansion coefficients through derivatives: two examples

The first of two steps that have led to the algorithm from (Cantero & Iserles 2011, Iserles 2011) is to represent the nth expansion coefficient in the form (1.3), as an infinite linear combination of derivatives at the origin. To this end we have first expressed x^n as a linear combination (1.2) of the first $n+1$ orthogonal polynomials, subsequently using analyticity in the neighbourhood of the support of the measure to construct the desired representation of expansion coefficients.

Similar results can be derived by direct calculation for other classical orthogonal polynomials. We first consider the *Hermite polynomials*

$$\mathrm{H}_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k n! (2x)^{n-2k}}{k!(n-2k)!}$$

(Rainville 1960, p. 187).

Lemma 1 *It is true that*

$$x^n = \frac{n!}{2^n} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{\mathrm{H}_{n-2k}(x)}{k!(n-2k)!}, \qquad n \in \mathbb{Z}_+. \tag{2.1}$$

Proof The assertion follows easily from the above explicit form of Hermite polynomials,

$$\begin{aligned}
&\frac{n!}{2^n} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{1}{k!(n-2k)!} \mathrm{H}_{n-2k}(x) = \frac{n!}{2^n} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{1}{k!} \sum_{m=0}^{\lfloor n/2 \rfloor - k} \frac{(-1)^m (2x)^{n-2k-2m}}{m!(n-2k-2m)!} \\
&= \frac{n!}{2^n} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{1}{k!} \sum_{m=k}^{\lfloor n/2 \rfloor} \frac{(-1)^{m-k} (2x)^{n-2m}}{(m-k)!(n-2m)!} \\
&= \frac{n!}{2^n} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(-1)^m (2x)^{n-2m}}{(n-2m)! m!} \sum_{k=0}^{m} (-1)^k \binom{m}{k} = \frac{n!}{2^n} \frac{(2x)^n}{n!} = x^n.
\end{aligned}$$

The identity (2.1) rapidly leads to the explicit representation of Hermite expansion coefficients in terms of derivatives: given an analytic function $f(x) = \sum_{n=0}^{\infty} f_n/n! x^n$, it follows from (2.1) that

$$
\begin{aligned}
f(x) &= \sum_{n=0}^{\infty} f_n \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{\mathrm{H}_{n-2k}(x)}{2^n k!(n-2k)!} \\
&= \sum_{n=0}^{\infty} \frac{f_{2n}}{2^{2n}} \sum_{k=0}^{n} \frac{\mathrm{H}_{2k}(x)}{(n-k)!(2k)!} + \sum_{n=0}^{\infty} \frac{f_{2n+1}}{2^{2n+1}} \sum_{k=0}^{n} \frac{\mathrm{H}_{2k+1}(x)}{(n-k)!(2k+1)!} \\
&= \sum_{k=0}^{\infty} \frac{1}{(2k)!} \sum_{n=k}^{\infty} \frac{f_{2n}\mathrm{H}_{2k}(x)}{2^{2n}(n-k)!} + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} \sum_{n=k}^{\infty} \frac{f_{2n+1}\mathrm{H}_{2k+1}(x)}{2^{2n+1}(n-k)!} \\
&= \sum_{k=0}^{\infty} \frac{1}{(2k)!} \sum_{n=0}^{\infty} \frac{f_{2n+2k}\mathrm{H}_{2k}(x)}{n! 2^{2n+2k}} + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} \sum_{n=0}^{\infty} \frac{f_{2n+2k+1}\mathrm{H}_{2k+1}(x)}{2^{2n+2k+1} n!}.
\end{aligned}
$$

□

A consequence of (2.1) is that

$$
\hat{f}_n = \frac{1}{2^n n!} \sum_{m=0}^{\infty} \frac{f^{(n+2m)}(0)}{2^{2m} m!(n+2m)!}, \qquad n \in \mathbb{Z}_+.
$$

Another important instance of an OPRL system is of generalized *Laguerre polynomials*

$$
\mathrm{L}_n^{(\alpha)}(x) = \frac{(1+\alpha)_n}{n!} \sum_{m=0}^{n} \frac{(-n)_m}{m!(1+\alpha)_m} x^m, \qquad n \in \mathbb{Z}_+,
$$

where $\alpha > 0$ (Rainville 1960, p. 200).

Lemma 2 *The representation (1.2) for Laguerre polynomials is*

$$
x^n = \sum_{m=0}^{n} (-1)^m \frac{n!(m+1+\alpha)_{n-m}}{(n-m)!} \mathrm{L}_m^{(\alpha)}(x), \qquad n \in \mathbb{Z}_+. \tag{2.2}
$$

Proof We wish to prove that $d_{n,m} = (-1)^m \frac{n!(m+\alpha+1)_{n-m}}{(n-m)!}$, $0 \le m \le n$. Since

$$
\begin{aligned}
x^n &= \sum_{m=0}^{n} d_{n,m} \mathrm{L}_m^{(\alpha)}(x) = \sum_{m=0}^{n} d_{n,m} (1+\alpha)_m \sum_{k=0}^{m} \frac{(-1)^k}{(m-k)!(1+\alpha)_k} x^k \\
&= \sum_{k=0}^{n} \frac{(-1)^k}{k!} \left[\sum_{m=0}^{n-k} d_{n,m+k} \frac{(k+1+\alpha)_m}{m!} \right] x^k
\end{aligned}
$$

and $d_{n,n} = (-1)^n n!$, (2.2) follows from

$$
\sum_{m=0}^{n-k} d_{n,m+k} \frac{(k+1+\alpha)_m}{m!} = 0, \qquad k = 0, 1, \ldots, n-1.
$$

This, however, can be verified easily. Letting $p = n - k = 1, 2, \ldots, n$,

$$\begin{aligned}
&\sum_{m=0}^{p} d_{n,m+n-p} \frac{(n-p+\alpha+1)_m}{m!} \\
&= (-1)^{p+n} n! \sum_{m=0}^{p} (-1)^m \frac{(n-p+\alpha+1)_m (m+n-p+\alpha+1)_{p-m}}{m!(p-m)!} \\
&= (-1)^{p+n} \frac{n!(n-p+\alpha+1)_p}{p!} \sum_{m=0}^{p} (-1)^m \binom{p}{m} = 0.
\end{aligned}$$

Therefore

$$\begin{aligned}
f(x) &= \sum_{n=0}^{\infty} \frac{f_n}{n!} x^n = \sum_{n=0}^{\infty} f_n \sum_{m=0}^{n} (-1)^m \frac{(m+\alpha+1)_{n-m}}{(n-m)!} \mathrm{L}_m^{(\alpha)}(x) \\
&= \sum_{m=0}^{\infty} (-1)^m \sum_{n=0}^{\infty} f_{n+m} \frac{(m+\alpha+1)_n}{n!} \mathrm{L}_n^{(\alpha)}(x).
\end{aligned}$$

□

The representation (1.3) for Laguerre polynomials is thus

$$\hat{f}_n = (-1)^n \sum_{m=0}^{\infty} \frac{(n+\alpha+1)_m f^{(n+m)}(0)}{m!(n+m)!}, \qquad n \in \mathbb{Z}_+.$$

2.2 Expansion coefficients through derivatives: general theory

For ultraspherical, Hermite and Laguerre polynomials we can evaluate the $d_{n,m}$s by brute force, but this clearly will not do for a general OPRL. Thus, we require a theory that represents the $d_{n,m}$s in a more organised manner.

Let $\{p_n\}_{n\in\mathbb{Z}_+}$ be a system of *monic* OPRLs with respect to the real Borel measure $\mathrm{d}\mu$. Hence

$$\int_{-\infty}^{\infty} p_m(x) p_n(x)\, \mathrm{d}\mu(x) = \begin{cases} \lambda_n > 0, & m = n, \\ 0, & m \neq n, \end{cases} \qquad m, n \in \mathbb{Z}_+.$$

Moreover, the p_ns obey a three-term recurrence relation of the form

$$p_{n+1}(x) = (x - a_n) p_n(x) - b_n p_{n-1}(x), \qquad n \in \mathbb{Z}_+, \tag{2.3}$$

where $p_{-1} \equiv 0$, $b_0 = 0$ and $b_n > 0$, $n \in \mathbb{N}$.

Since $p_0, p_1, \ldots, p_n$ form the basis of the linear space of nth-degree polynomials, for every $n \in \mathbb{Z}_+$ there exist real constants $d_{n,m}$ such that

$$x^n = \sum_{m=0}^{n} d_{n,m} p_m(x).$$

The constants $d_{n,m}$ can be obtained at once from (1.1),

$$d_{n,m} = \frac{1}{\lambda_m} \int_{-\infty}^{\infty} x^n p_m(x)\,\mathrm{d}\mu(x), \qquad m = 0, 1, \ldots, n.$$

Substituting this into the recurrence relation (2.3), we obtain

$$d_{n+1,m} = \frac{1}{\lambda_m}(\lambda_{m-1} b_m d_{n,m-1} + \lambda_m a_m d_{n,m} + \lambda_{m+1} d_{n,m+1}), \quad m = 0, 1, \ldots, n,\ n \in \mathbb{Z}_+.$$

This expression can be somewhat beautified by letting $\tilde{d}_{n,m} = \lambda_m d_{n,m}/\lambda_0$, whereby

$$\tilde{d}_{n+1,m} = b_m \tilde{d}_{n,m-1} + a_m \tilde{d}_{n,m} + \tilde{d}_{n,m+1}, \qquad m, n \in \mathbb{Z}_+, \tag{2.4}$$

where we have let $\tilde{d}_{n,m} = 0$ for $m \geq n+1$.

The recurrence (2.4) can be written in a more compact form using vector notation. Thus, letting

$$\boldsymbol{d}_n = \begin{bmatrix} \tilde{d}_{n,0} \\ \tilde{d}_{n,1} \\ \tilde{d}_{n,2} \\ \vdots \end{bmatrix}, \quad n \in \mathbb{Z}_+, \qquad \mathcal{H} = \begin{bmatrix} a_0 & 1 & 0 & \cdots & \cdots \\ b_1 & a_1 & 1 & \ddots & \\ 0 & b_2 & a_2 & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

we have $\boldsymbol{d}_0 = \boldsymbol{e}_0$, the zeroth coordinate vector, and $\boldsymbol{d}_{n+1} = \mathcal{H}\boldsymbol{d}_n$, $n \in \mathbb{Z}_+$. Therefore

$$\boldsymbol{d}_n = \mathcal{H}^n \boldsymbol{e}_0, \qquad n \in \mathbb{Z}_+. \tag{2.5}$$

Let $\mathcal{S}$ be the infinite diagonal matrix, indexed by $\mathbb{Z}_+$, with $\mathcal{S}_{0,0} = 1$ and $\mathcal{S}_{m,m} = (b_1 b_2 \cdots b_m)^{1/2}$, $m \in \mathbb{N}$ (recall that $b_m > 0$). Then

$$\mathcal{S}^{-1}\mathcal{H}\mathcal{S} = \mathcal{J} = \begin{bmatrix} a_0 & b_1^{1/2} & 0 & \cdots & \cdots \\ b_1^{1/2} & a_1 & b_2^{1/2} & \ddots & \\ 0 & b_2^{1/2} & a_2 & b_3^{1/2} & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

Note that $\mathcal{J}$ is the *Jacobi matrix* of the OPRL system $\{p_n\}_{n\in\mathbb{Z}_+}$. We note for further reference that the essential spectrum of $\mathcal{J}$, hence also of $\mathcal{H}$ coincides, subject to very generous conditions, with the support of the measure $\mathrm{d}\mu$ (Chihara 1978).

2.3 Expansion coefficients through the Cauchy Integral Theorem

The second step in the 'grand scheme' of Section 1 is to express expansion coefficients $\hat{f}_n$, $n \in \mathbb{Z}_+$, using the Cauchy integral theorem. To this end we assume that the support Γ of $\mathrm{d}\mu$ is the finite interval (a,b) and that $0\in[a,b]$.[1] Let γ be a simple Jordan curve in $\mathbb{C}\setminus[a,b]$ with winding number one and assume that the function

$$f(z)=\sum_{m=0}^{\infty} f_m z^m, \qquad f_m=\frac{f^{(m)}(0)}{m!}, \quad m\in\mathbb{Z}_+,$$

is analytic on and inside γ. According to our definition of $\tilde{d}_{n,m}$ we have

$$f(z)=\sum_{m=0}^{\infty} f_m z^m=\sum_{m=0}^{\infty} f_m \sum_{n=0}^{m} d_{m,n}p_n(z)=\sum_{n=0}^{\infty}\sum_{m=n}^{\infty} f_m d_{m,n}p_n(z),$$

therefore

$$\hat{f}_n=\frac{\lambda_0}{\lambda_n}\sum_{m=n}^{\infty} f_m\tilde{d}_{m,n}=\frac{\lambda_0}{\lambda_n}\sum_{m=n}^{\infty}\frac{f^{(m)}(0)}{m!}\tilde{d}_{m,n}=\frac{\lambda_0}{\lambda_n}\frac{1}{2\pi\mathrm{i}}\int_\gamma f(z)\sum_{m=n}^{\infty}\frac{\tilde{d}_{m,n}}{z^{m+1}}\,\mathrm{d}z.$$

According to (2.5) it is true that $\tilde{d}_{m,n}=\boldsymbol{e}_n^\top\mathcal{H}^m\boldsymbol{e}_0$, $m,n\in\mathbb{Z}_+$, therefore

$$\sum_{m=n}^{\infty}\frac{\tilde{d}_{m,n}}{z^{n+1}}=\frac{1}{z}\boldsymbol{e}_n^\top\left(\sum_{m=n}^{\infty}\mathcal{H}^m z^{-m}\right)\boldsymbol{e}_0=\frac{1}{z^{n+1}}\boldsymbol{e}_n^\top\mathcal{H}^n(I-z^{-1}\mathcal{H})^{-1}\boldsymbol{e}_0, \qquad n\in\mathbb{Z}_+.$$

We deduce that

$$\hat{f}_n=\frac{\lambda_0}{\lambda_n}\frac{1}{2\pi\mathrm{i}}\int_\gamma\frac{f(z)}{z^{n+1}}\boldsymbol{e}_n^\top\mathcal{H}^n(I-z^{-1}\mathcal{H})^{-1}\boldsymbol{e}_0\,\mathrm{d}z, \qquad n\in\mathbb{Z}_+. \tag{2.6}$$

Following upon our former remark, the essential spectrum of $\mathcal{H}$ being restricted to $[a,b]$, we deduce that the resolvent $(I-z^{-1}\mathcal{H})^{-1}$ is analytic on γ, hence the integral in (2.6) is well defined.

To make deeper sense of (2.6), let us denote by $\mathcal{H}_N$ the $N\times N$ section of the infinite matrix $\mathcal{H}$, therefore $p_N(z)=\det(zI-\mathcal{H}_N)$. Then, choosing large N and denoting by $\operatorname{adj}A$ the *adjunct* of the matrix A,

$$\hat{f}_0\approx\frac{1}{2\pi\mathrm{i}}\int_\gamma\frac{f(z)}{z}\boldsymbol{e}_0^\top(I-z^{-1}\mathcal{H}_N)^{-1}\boldsymbol{e}_0\,\mathrm{d}z=\frac{1}{2\pi\mathrm{i}}\int_\gamma\frac{f(z)}{z}\frac{\boldsymbol{e}_0^\top\operatorname{adj}(I-z^{-1}\mathcal{H}_N)\boldsymbol{e}_0}{z^{-N}p_N(z)}\,\mathrm{d}z.$$

It is trivial to verify that $\boldsymbol{e}_0^\top(I-z^{-1}\mathcal{H}_N)\boldsymbol{e}_0$ is nothing else but the determinant of $I-z^{-1}\mathcal{H}_N$, with the first row and column excised. This, in turn equals $z^{-N+1}p_{N-1}^{(1)}$, where $p_n^{(1)}$ is the first (monic) *numerator polynomial* (also known as associated orthogonal polynomials) (Chihara 1978, p. 87) of the OPRL system $\{p_n\}$. Since

$$\frac{p_{N-1}^{(1)}(z)}{p_N(z)}=\sum_{k=1}^{N}\frac{b_k^{[N]}}{z-\xi_k^{[N]}},$$

[1] Without loss of generality and to simplify matters, we expand about the origin.

where $\xi_1^{[N]}, \xi_2^{[N]}, \ldots, \xi_N^{[N]} \in (a,b)$ and $b_1^{[N]}, b_2^{[N]}, \ldots, b_N^{[N]}$ are the nodes and the weights of the N-point Gauss–Christoffel quadrature formula corresponding to the Borel measure $\mathrm{d}\mu$ (Chihara 1978, p. 88), we deduce from the Cauchy integral theorem that

$$\hat{f}_0 \approx \sum_{k=1}^{N} \frac{b_k^{[N]}}{2\pi\mathrm{i}} \int_\gamma \frac{f(z)}{z-\xi_k^{[N]}}\,\mathrm{d}z = \sum_{k=1}^{N} b_k^{[N]} f(\xi_k^{[N]}).$$

Letting $N \to \infty$ we obtain an alternative proof of (2.6) in the special case $n = 0$.

Proceeding similarly for general $n \in \mathbb{Z}_+$, we have

$$\hat{f}_n \approx \frac{\lambda_0}{\lambda_n} \frac{1}{2\pi\mathrm{i}} \int_\gamma \frac{f(z)}{z^{n+1}} \frac{\boldsymbol{e}_n^\top \mathcal{H}_N^n \mathrm{adj}\,(I - z^{-1}\mathcal{H})\boldsymbol{e}_0}{z^{-N} p_N(z)}\,\mathrm{d}z. \tag{2.7}$$

In particular, for $n = 1$ direct computation affirms that

$$\begin{aligned} &\boldsymbol{e}_1^\top \mathcal{H}_N \mathrm{adj}\,(I - z^{-1}\mathcal{H})\boldsymbol{e}_0 \\ &= b_1 \mathrm{adj}(I - z^{-1}\mathcal{H}_N)_{0,0} + a_1 \mathrm{adj}(I - z^{-1}\mathcal{H}_N)_{1,0} + \mathrm{adj}(I - z^{-1}\mathcal{H}_N)_{2,0}. \end{aligned}$$

Moreover,

$$\begin{aligned} \mathrm{adj}(I - z^{-1}\mathcal{H}_N)_{0,0} &= z^{-N+1} p_{N-1}^{(1)}(z), \\ \mathrm{adj}(I - z^{-1}\mathcal{H}_N)_{1,0} &= b_1 z^{-N+1} p_{N-2}^{(2)}(z), \\ \mathrm{adj}(I - z^{-1}\mathcal{H}_N)_{2,0} &= b_1 b_2 z^{-N+1} p_{N-3}^{(3)}(z), \end{aligned}$$

where $p_n^{(k)}$ is the kth numerator polynomial: Each $\{p_n^{(k)}\}_{n\in\mathbb{Z}_+}$ is an OPRL system with the recurrence relation

$$p_{n+1}^{(k)}(x) = (x - a_{n+k}) p_n^{(k)}(x) - b_{n+k} p_{n-1}^{(k)}(x), \qquad n \in \mathbb{Z}_+$$

(Chihara 1978, p. 88) – compare with (2.3). Thus,

$$\boldsymbol{e}_1^\top \mathcal{H}_N \mathrm{adj}\,(I - z^{-1}\mathcal{H}_N)\boldsymbol{e}_0 = b_1 z^{-N+1}[p_{N-1}^{(1)}(z) + a_1 p_{N-2}^{(2)}(z) + b_2 p_{N-3}^{(3)}(z)].$$

Expanding the determinantal representation of $p_{N-1}^{(1)}$ in leading row and column, it is easy to prove that

$$p_{N-1}^{(1)}(z) = (z - a_1) p_{N-2}^{(2)}(z) - b_2 p_{N-3}^{(3)}(z),$$

and this results in $\boldsymbol{e}_1^\top \mathcal{H}_N \mathrm{adj}\,(I - z^{-1}\mathcal{H}_N)\boldsymbol{e}_0 = b_1 z^{-N+2} p_{N-2}^{(2)}(z)$ and, substituting in (2.7),

$$\hat{f}_1 \approx \frac{\lambda_0}{\lambda_1} \frac{b_1}{2\pi\mathrm{i}} \int_\gamma f(z) \frac{p_{N-2}^{(2)}(z)}{p_N(z)}\,\mathrm{d}z.$$

This connection between expansion coefficients and numerator polynomials, which can be probably generalised to all values of $n \in \mathbb{Z}_+$, is interesting on its own merit, although it adds little to our main purpose, the design of fast means to compute expansion coefficients. To this end the interesting expression is (2.6).

Naive computation of (2.6) is based on truncating the Taylor expansion of $I - z^{-1}\mathcal{H}$. Thus, given $M \in \mathbb{Z}_+$, we may approximate

$$\begin{aligned}\hat{f}_n &\approx \frac{\lambda_0}{\lambda_n}\frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{n+1}}\boldsymbol{e}_n^\top \sum_{m=n}^{n+M}\mathcal{H}^m z^{-m}\boldsymbol{e}_0\,\mathrm{d}z\\ &= \frac{\lambda_0}{\lambda_n}\sum_{m=n}^{n+M}\boldsymbol{e}_n^\top\mathcal{H}^m\boldsymbol{e}_0\frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{n+m+1}}\,\mathrm{d}z, \qquad n \in \mathbb{Z}_+. \end{aligned} \tag{2.8}$$

The coefficients $\beta_{n,m} = \boldsymbol{e}_n^\top \mathcal{H}^m \boldsymbol{e}_0$ can be computed rapidly by recursion, using the three-term recurrence relation (2.6). Moreover, provided that we can choose a circular trajectory γ, the integrals can be computed with FFT. Therefore it might seem that we have recovered a generalisation of the 'fast ultraspherical approximation' from (Cantero & Iserles 2011) to the realm of arbitrary OPRL systems on compact intervals.

Unfortunately, because of slow convergence of truncated Taylor series in (2.8), the algorithm requires $M = \mathcal{O}(N)$ to compute $\hat{f}_n$, $n = 0, 1, \ldots, N-1$, to any given tolerance, and this results in an $\mathcal{O}\bigl(N^2\bigr)$ method. Like in the case of ultraspherical polynomials, the main hope in harnessing (2.6) toward rapid computation of expansion coefficients lies in an appropriate transformation, converting $\{\beta_{n,m}\}_{m=N}^{n+M}$ into a rapidly convergent sequence. This might be accomplished either by a serendipitous formula *á la* (Cantero & Iserles 2011) or perhaps, with greater generality, by a general method for the acceleration of convergence of sequences (Sidi 2003). All this is matter for future exploration.

2.4 Chebyshev polynomials of the second kind

In general, there is little prospect of manipulating (2.6) directly to recover (1.5) in the case of ultraspherical polynomials. An exception is the case $\alpha = \frac{1}{2}$, corresponding to $\{\mathrm{U}_n\}_{n\in\mathbb{Z}_+}$, Chebyshev polynomials of the second kind. Recall that $\mathrm{U}_n = (n+1)!/(\frac{3}{2})_n \mathrm{P}_n^{(1/2,1/2)}$. Moreover, $\mathrm{U}_n(x) = 2^n x^n + \text{l.o.t.}$ (Rainville 1960), hence $\tilde{\mathrm{U}}_n = 2^{-n}\mathrm{U}_n$, $n \in \mathbb{Z}_+$, are monic. Therefore, expanding in the U_ns, rather than in $\mathrm{P}_n^{(1/2,1/2)}$s, (1.5) becomes

$$\tilde{K}_n(z) = {}_2\mathrm{F}_1\left[\begin{matrix}\frac{n+1}{2}, \frac{n+2}{2};\\ n+2;\end{matrix}\ \frac{1}{z^2}\right], \qquad n \in \mathbb{Z}_+. \tag{2.9}$$

Our challenge is to recover (2.9) directly from (2.6). First, however, we note that $\lambda_n = 2^{-n-1}\pi$, $n \in \mathbb{Z}_+$, since it is trivial to show, e.g. from the identity $\mathrm{U}_n(\cos\theta) = \sin((n+1)\theta)/\sin\theta$, that $\int_{-1}^1 \mathrm{U}_n^2(x)(1-x^2)^{1/2}\,\mathrm{d}x \equiv \pi/2$.

The reason our task is at all possible is that $\mathcal{H}$ is a Toeplitz matrix, because $a_n \equiv 0$ and $b_n \equiv \frac{1}{4}$. Recalling that $\tilde{d}_{r,s} = \boldsymbol{e}_r^\top \mathcal{H}^s \boldsymbol{e}_0 = 2^{-s}\boldsymbol{e}_r^\top \mathcal{J}^s \boldsymbol{e}_0$, we deduce that $\tilde{d}_{r,s} = 4^{-s} v_{r,s}$, where

$$v_{r,s} = \boldsymbol{e}_r^\top \tilde{J}^s \boldsymbol{e}_0, \quad r, s, \in \mathbb{Z}_+, \qquad \text{where} \qquad \tilde{\mathcal{J}} = \begin{bmatrix} 0 & 1 & 0 & \cdots & \cdots \\ 1 & 0 & 1 & \ddots & \\ 0 & 1 & 0 & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

We wish to determine the explicit form of the $v_{r,s}$s. Our first step, surprisingly non-trivial, is to determine $v_{0,2s}$: it is trivial that $v_{0,2s+1}=0$. Let us denote by $\tilde{\mathcal{J}}^{(n)}$ the $n\times n$ section of the infinite-dimensional matrix $\mathcal{J}$. Then $\tilde{\mathcal{J}}^{(n)}=\mathcal{Q}^{(n)}\Lambda^{(n)}\mathcal{Q}^{(n)}$, where $\mathcal{Q}^{(n)}$ is an orthogonal symmetric matrix, $\tilde{Q}^{(n)}_{k,l}=(2/n)^{1/2}\sin\frac{\pi kl}{n}$, while $\Lambda^{(n)}$ is diagonal, $\Lambda^{(n)}_{k,k}=2\cos\frac{k\pi}{n}$ (Iserles 2009). $\tilde{\mathcal{J}}$ is a Hermitian Toeplitz matrix. Therefore, as the consequence of the Grenander–Szegő theorem (Grenender & Szegő 1958), it is true that

$$\lim_{n\to\infty}\boldsymbol{e}_r^{(n)\top}\tilde{\mathcal{J}}^{(n)s}\boldsymbol{e}_0^{(n)}=\boldsymbol{e}_r^\top\mathcal{J}^s\boldsymbol{e}_0,\qquad r,s\in\mathbb{Z}_+,$$

where $\boldsymbol{e}_r^{(n)}\in\mathbb{R}^n$ is the rth unit vector. But

$$\begin{aligned}\boldsymbol{e}_0^{(n)\top}\tilde{\mathcal{J}}^{(n)2s}\boldsymbol{e}_0^{(n)} &= \boldsymbol{e}_0^{(n)\top}\mathcal{Q}^{(n)}\Lambda^{(n)2s}\mathcal{Q}^{(n)}\boldsymbol{e}_0^{(n)}=\frac{2^{2s+1}}{n}\sum_{k=0}^{n-1}\sin^2\tfrac{k\pi}{n}\cos^{2s}\tfrac{k\pi}{n}\\ &\overset{n\to\infty}{\longrightarrow} 2^{2s+1}\int_0^1\sin^2\pi x\cos^{2s}\pi x\,\mathrm{d}x\\ &= 2^{2s+1}\left[\int_0^1\cos^{2s}\pi x\,\mathrm{d}x-\int_0^1\cos^{2(s+1)}\pi x\,\mathrm{d}x\right].\end{aligned}$$

Since trivial calculation confirms that

$$\int_0^1\cos^{2s}\pi x\,\mathrm{d}x=\frac{1}{4^s}\binom{2s}{s},\qquad s\in\mathbb{Z}_+,$$

it is now easy to deduce that

$$v_{0,2s}=\frac{(2s)!}{s!(s+1)!},\qquad s\in\mathbb{Z}_+.$$

Next we observe that $v_{1,s+1}=(\tilde{\mathcal{J}}\boldsymbol{e}_1)^\top\tilde{\mathcal{J}}^s\boldsymbol{e}_0=\boldsymbol{e}_0^\top\tilde{\mathcal{J}}^s\boldsymbol{e}_0$, therefore $v_{1,2s}=0$ and $v_{1,2s+1}=(2s)!/[s!(s+1)!]$, $s\in\mathbb{Z}_+$. We continue by induction on r. For any $r,s\in\mathbb{N}$ it is true that

$$v_{r,s}=(\tilde{\mathcal{J}}\boldsymbol{e}_r)^\top\tilde{\mathcal{J}}^{s-1}\boldsymbol{e}_0=(\boldsymbol{e}_{r-1}+\boldsymbol{e}_{r+1})^\top\mathcal{J}^{s-1}\boldsymbol{e}_0=v_{r-1,s-1}+v_{r+1,s-1}.\tag{2.10}$$

Our assertion is that, for every $r,s\in\mathbb{Z}_+$,

$$\begin{aligned}v_{2r,2s} &= (-1)^r(2r+1)\frac{(-s)_r(2s)!}{s!(s+r+1)!}, && v_{2r,2s+1}=0,\\ v_{2r+1,2s} &= 0, && v_{2r+1,2s+1}=(-1)^r(r+1)\frac{(-s)_r(2s+2)!}{(s+1)!(s+r+2)!}.\end{aligned}\tag{2.11}$$

This is certainly consistent with $r=0,1$, while for $r\geq 2$ the result follows by induction, substituting into (2.10).

We now have all the ingredients necessary to construct $\tilde{K}_n$. Note that

$$\tilde{K}_n(z)=\frac{\lambda_0}{\lambda_n}\sum_{m=n}^{\infty}\tilde{d}_{n,m}z^{m-n}=4^n\sum_{m=0}^{\infty}\tilde{d}_{n,m+n}z^{-m}=\sum_{m=0}^{\infty}2^{-m}v_{n,m+n}z^{-m}.$$

Therefore,

$$\begin{aligned}\tilde{K}_{2n}(z) &= (-1)^n(2n+1)\sum_{m=0}^{\infty}\frac{(-n-m)_n(2n+2m)!}{(n+m)!(2n+m+1)!}\frac{1}{(2z)^{2m}}\\ &= (2n+1)\sum_{m=0}^{\infty}\frac{1}{m!}\frac{(2n+2m)!}{(2n+m+1)!}\frac{1}{(2z)^{2m}}.\end{aligned}$$

But

$$\begin{aligned}\frac{(2n+1)(2n+2m)!}{(2n+m+1)!} &= \frac{(2n+2m)!}{(2n)!(2n+2)_m} = \frac{(2n+1)_{2m}}{(2n+2)!}\\ &= \frac{[(n+\frac{1}{2})(n+\frac{3}{2})\cdots(n+m-\frac{1}{2})]\cdot[(n+1)(n+2)\cdots(n+m)]}{4^{-m}(2n+2)_m}\\ &= \frac{(n+\frac{1}{2})_m(n+1)_m}{4^{-m}(2n+2)_m},\end{aligned}$$

therefore

$$\tilde{K}_{2n}(z) = \sum_{m=0}^{\infty}\frac{(n+\frac{1}{2})_m(n+1)_m}{m!(2n+2)_m}z^{-2m} = {}_2\mathrm{F}_1\left[\begin{matrix} n+\frac{1}{2}, n+1; & \frac{1}{z^2} \\ 2n+2; & \end{matrix}\right],$$

consistently with (2.9). Likewise,

$$\begin{aligned}\tilde{K}_{2n+1}(z) &= (-1)^n(n+1)\sum_{m=0}^{\infty}\frac{(-n-m)_n(2n+2m+1)!}{(n+m+1)!(2n+2m+2)!}\frac{1}{(2z)^m}\\ &= \sum_{m=0}^{\infty}\frac{(n+1)!(n+\frac{3}{2})_n}{m!(2n+3)!}\frac{1}{z^{2m}} = {}_2\mathrm{F}_1\left[\begin{matrix} n+1, n+\frac{3}{2}; & \frac{1}{z^2} \\ 2n+3; & \end{matrix}\right]\end{aligned}$$

and, again, we deduce (2.5).

3 Orthogonal polynomials on the unit circle

3.1 Expansion coefficients through derivatives: general theory

We commence by reviewing elements of the theory of orthogonal polynomials on the unit circle, referring the reader to (Geronimus 1961, Simon 2005, Simon 2007, Szegő 1975) for further details.

Let μ be a measure supported on the unit circle and denote by $\mathbb{P} = \mathbb{C}[z]$ the linear space of polynomials with complex coefficients and by $\mathbb{P}_n$ the subspace of polynomials with degree less or equal n. $\Lambda := \mathbb{C}[z, z^{-1}]$ denotes the complex vector subspace of Laurent polynomials and $\Lambda_{m,n} := \mathrm{Span}\{z^m, z^{m+1}, \ldots, z^n\}$ for $m \le n$, $m, n \in \mathbb{Z}$. We consider the inner product

$$\langle p, q\rangle_\mu = \int_{\mathbb{T}} p(z)\bar{q}(z^{-1})\,\mathrm{d}\mu(z), \qquad p, q \in \Lambda,$$

where $\mathbb{T}$ is the complex unit circle. It is clear that it satisfies the property

$$\langle zp(z), zq(z)\rangle_\mu = \langle p(z), q(z)\rangle_\mu \qquad \forall p, q \in \Lambda.$$

Applying the Gram–Schmidt orthogonalization procedure over the canonical basis $\{z^n\}_{n\geq 0}$, we obtain the corresponding sequence $(p_n)_{n\geq 0}$ of *orthogonal polynomials on the unit circle (OPUC)*. Specifically,

(i) $p_n \in \mathbb{P}_n \setminus \mathbb{P}_{n-1}$.

(ii) $\langle p_n, z^k\rangle = 0$, $k = 0, 1, \ldots, n-1$.

In what follows we will denote by $\{\phi_n\}_{n\geq 0}$ the sequence of monic OPUC and let $\kappa_n = 1/\|\phi_n\||_\mu$. It is very well known that the OPUC satisfy the three terms recurrence relation

$$\phi_n(z) = z\phi_{n-1}(z) + a_n\phi^*_{n-1}(z), \tag{3.1}$$

where $\phi^*_n(z) := z^n\bar{\phi}_n(z^{-1})$ is the so-called *reciprocal polynomial* (Simon 2005). The numbers $a_n = \phi_n(0)$ are called *Schur parameters* or *Verblunsky coefficients*. Note that $|a_n| < 1$ for $n \in \mathbb{N}$. Straightforward calculation demonstrates that

$$\frac{\kappa^2_{n-1}}{\kappa^2_n} = 1 - |a_n|^2, \qquad n \in \mathbb{N}.$$

The recurrence relation (3.1) gives ϕ_n in terms of ϕ_{n-1} and ϕ^*_{n-1}. Acting with the operator $*$ for polynomials of degree n in both sides of (3.1) results in

$$\phi^*_n(z) = \bar{a}_n z\phi_{n-1}(z) + \phi^*_{n-1}(z). \tag{3.2}$$

We eliminate ϕ^*_{n-1} from (3.1) and (3.2), the outcome being

$$\phi_n(z) - a_n\phi^*_n(z) = (1 - |a_n|^*)z\phi_{n-1}(z). \tag{3.3}$$

Writing (3.1) for $n+1$ and substituting in (3.3), we finally obtain

$$(a_{n+1} + a_n z)\phi_n(z) = a_n\phi_{n+1}(z) + (1 - |a_n|^2)a_{n+1}z\phi_{n-1}(z) \tag{3.4}$$

an order-two difference equation for the OPUC.

Taking the polynomials $(\phi_n)_{n\geq 0}$ as a basis, there necessarily exist $d_{n,m}$, $m = 0, 1, \ldots, n$, such that

$$z^n = \sum_{m=0}^{n} d_{n,m}\phi_m(z), \qquad n \in \mathbb{Z}_+.$$

The coefficients $d_{n,m}$ can be obtained from

$$\langle z^n, \phi_l\rangle = \sum_{m=0}^{n} d_{n,m}\langle\phi_m, \phi_l\rangle, \qquad l = 0, 1, \ldots, n,$$

implying that

$$\|\phi_m\|^2_\mu d_{n,m} = \int_{\mathbb{T}} z^n\bar{\phi}_m(z^{-1})\,\mathrm{d}\mu(z).$$

We suppose that $a_m \in \mathbb{C}$ is nonzero for all $m \in \mathbb{Z}_+$. (Recall that if $a_m = 0$ for all $m \in \mathbb{Z}_+$ then the corresponding sequence $\{\phi_n\}_{n\in\mathbb{Z}_+}$ corresponds to orthogonal polynomials with respect to the usual Lebesgue measure on the unit circle, $\phi_n(z) = z^n$.) Therefore, multiplying (3.4) (with n replaced by m) by z^n and integrating along the unit circle,

$$\begin{aligned}&\bar{a}_{m+1}\|\phi_m\|_\mu^2 d_{n,m} + \bar{a}_m\|\phi_m\|_\mu^2 d_{n-1,m}\\ &= \bar{a}_m\|\phi_{m+1}\|_\mu^2 d_{n,m+1} + (1-|a_m|^2)\bar{a}_{m+1}\|\phi_{m-1}\|_\mu^2 d_{n-1,m-1}\end{aligned}$$

– equivalently

$$d_{n,m} - \frac{\bar{a}_m}{\bar{a}_{m+1}}\frac{\|\phi_{m+1}\|_\mu^2}{\|\phi_m\|_\mu^2} d_{n,m+1} = (1-|a_m|^2)\frac{\|\phi_{m-1}\|_\mu^2}{\|\phi_m\|_\mu^2} d_{n-1,m-1} - \frac{\bar{a}_m}{\bar{a}_{m+1}} d_{n-1,m}.$$

However,

$$(1-|a_m|^2)\frac{\|\phi_{m-1}\|_\mu^2}{\|\phi_m\|_\mu^2} = (1-|a_m|^2)\frac{\kappa_m^2}{\kappa_{m-1}^2} = 1,$$

therefore

$$d_{n,m} - \frac{\bar{a}_m}{\bar{a}_{m+1}}(1-|a_{m+1}|^2) d_{n,m+1} = d_{n-1,m-1} - \frac{\bar{a}_m}{\bar{a}_{m+1}} d_{n-1,m} \tag{3.5}$$

for $m \in \mathbb{Z}_+$, subject to the convention that $d_{n,-1} \equiv 1$. In matricial form we have

$$\mathcal{S}\boldsymbol{d}_{n+1} = \mathcal{T}\boldsymbol{d}_n.$$

$\boldsymbol{d}_n$ being the column vector $[d_{n,0}, d_{n,1}, d_{n,2}, \cdots]^\top$ with $d_{n,m} = 0$, $m \ge n+1$ and

$$\mathcal{S} = \begin{bmatrix} 1 & -\frac{\bar{a}_0}{\bar{a}_1}\rho_1^2 & 0 & 0 & 0 & \cdots \\ 0 & 1 & -\frac{\bar{a}_1}{\bar{a}_2}\rho_2^2 & 0 & 0 & \cdots \\ 0 & 0 & 1 & -\frac{\bar{a}_2}{\bar{a}_3}\rho_3^2 & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

$$\mathcal{T} = \begin{bmatrix} -\frac{\bar{a}_0}{\bar{a}_1} & 0 & 0 & 0 & \cdots \\ 1 & -\frac{\bar{a}_1}{\bar{a}_2} & 0 & 0 & \cdots \\ 0 & 1 & -\frac{\bar{a}_2}{\bar{a}_3} & 0 & \cdots \\ 0 & 0 & 1 & -\frac{\bar{a}_3}{\bar{a}_4} & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

where $\rho_n = (1-|a_n|^2)^{1/2}$: recall that $d_{n,-1} \equiv 0$. Denoting by $\mathcal{S}_n$ and $\mathcal{T}_n$ the principal submatrices of order n, of $\mathcal{S}$ and $\mathcal{T}$ respectively, and bearing in mind that $a_n \neq 0$ for all $n \in \mathbb{Z}_+$, we have

$$\boldsymbol{d}_{n+1} = \mathcal{S}_n^{-1}\mathcal{T}_n\boldsymbol{d}_n = \mathcal{H}\boldsymbol{d}_n,$$

where $\mathcal{H} = \mathcal{S}^{-1}\mathcal{T}$. Note that, like in Section 3, $\boldsymbol{d}_0 = \boldsymbol{e}_0$ and

$$\boldsymbol{d}_n = \mathcal{H}^n \boldsymbol{e}_0, \qquad n \in \mathbb{Z}_+. \tag{3.6}$$

Theorem 3 *$\mathcal{H}$ is an irreducible upper-Hessenberg matrix such that*

$$\mathcal{H}_{k,l} = \begin{cases} -\bar{a}_k a_{l+1} \displaystyle\prod_{j=k+1}^{l} \rho_j^2, & k \le l, \\ 1, & k = l+1, \\ 0, & k \ge l+2. \end{cases} \tag{3.7}$$

Proof Let

$$\mathcal{S} = \begin{bmatrix} 1 & -c_0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & -c_1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & -c_2 & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}, \qquad \mathcal{T} = \begin{bmatrix} -f_0 & 0 & 0 & 0 & \cdots \\ 1 & -f_1 & 0 & 0 & \cdots \\ 0 & 1 & -f_2 & 0 & \cdots \\ 0 & 0 & 1 & -f_3 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

It is trivial that $\mathcal{S}^{-1}$ is upper triangular and

$$(\mathcal{S}^{-1})_{k,k+m} = \prod_{j=k}^{k+m-1} c_j, \qquad k, m \in \mathbb{Z}_+.$$

The matrix $\mathcal{H}$ is clearly upper Hessenberg and $\mathcal{H}_{k+1,k} \equiv 1$, hence irreducibility. Moreover, for every $k, m \in \mathbb{Z}_+$

$$\begin{aligned} \mathcal{H}_{k,k+m} &= \sum_{j=0}^{\infty} (\mathcal{S}^{-1})_{k,j} \mathcal{T}_{j,k+m} = (\mathcal{S}^{-1})_{k,k+m} \mathcal{T}_{k+m,k+m} + (\mathcal{S}^{-1})_{k,k+m+1} \mathcal{T}_{k+m+1,k+m} \\ &= -\left(\prod_{j=k}^{k+m-1} c_j \right) f_{k+m} + \prod_{j=k}^{k+m} c_j = \left(\prod_{j=k}^{k+m-1} c_j \right) (c_{k+m} - f_{k+m}). \end{aligned}$$

In our case

$$c_j = \frac{\bar{a}_j}{\bar{a}_{j+1}} \rho_{j+1}^2, \quad f_j = \frac{\bar{a}_j}{\bar{a}_{j+1}}, \qquad j \in \mathbb{Z}_+,$$

therefore, telescoping a product,

$$\mathcal{H}_{k,k+m} = \left(\prod_{j=k}^{k+m} \rho_j^2 \right) \frac{\bar{a}_k}{\bar{a}_{k+m+1}} (\rho_{k+m+1}^2 - 1) = -\bar{a}_k a_{k+m+1} \prod_{j=k}^{k+m} \rho_j^2.$$

The proof is complete. □

The matrix $\mathcal{H}$ is not new and it plays an important role in OPUC theory (Simon 2005, p. 252). However, both its role in deriving the $\boldsymbol{d}_n$s and its representation as the product $\mathcal{S}^{-1}\mathcal{T}$ are new.

3.2 Two examples

OPUC being less well known than OPRL, it is helpful to illustrate our narrative with some examples. Firstly, we consider the sequence of orthogonal polynomials with respect to a measure $\mathrm{d}\mu(\theta) = (1-\cos\theta)\,\mathrm{d}\theta/(2\pi)$ defined on $\mathbb{T}$. In that case it is known that the sequence of monic polynomials $(\phi_n)_{n\in\mathbb{Z}_+}$ is given by

$$\phi_n(z) = \frac{1}{n+1}\sum_{j=0}^{n}(j+1)z^j$$

with the Schur parameters

$$a_n = \frac{1}{n+1},$$

and

$$\kappa_n = \sqrt{\frac{2(n+1)}{n+2}}, \qquad n \in \mathbb{Z}_+,$$

(Simon 2005), where we recall that $\kappa_n = 1/\|\phi_n\|_\mu$.

In this very simple case we do not need the theory of Subsection 4.1, since trivially

$$z^n = \phi_n(z) - \frac{n}{n+1}\phi_{n-1}(z), \qquad n \in \mathbb{N}.$$

Nonetheless, it is interesting to verify that the theory indeed delivers the right results.

It follows from (3.7) that

$$\mathcal{H}_{m,m-1} = 1, \qquad \mathcal{H}_{m,m+k} = -\frac{1}{(m+2)(m+k+1)}, \quad k \in \mathbb{Z}_+.$$

We prove $\boldsymbol{d}_n = \boldsymbol{e}_n - \frac{n}{n+1}\boldsymbol{e}_{n-1}$, $n \in \mathbb{N}$, by induction on n. Thus,

$$\mathcal{H}\boldsymbol{d}_n = \mathcal{H}\boldsymbol{e}_n - \frac{n}{n+1}\mathcal{H}\boldsymbol{e}_{n-1} = \begin{bmatrix} \mathcal{H}_{0,n} \\ \mathcal{H}_{1,n} \\ \vdots \\ \mathcal{H}_{n,n} \\ \mathcal{H}_{n+1,n} \\ 0 \\ \vdots \end{bmatrix} - \frac{n}{n+1}\begin{bmatrix} \mathcal{H}_{0,n-1} \\ \mathcal{H}_{1,n-1} \\ \vdots \\ \mathcal{H}_{n,n-1} \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

and

$$\begin{aligned} d_{n+1,n+1} &= \mathcal{H}_{n+1,n} = 1, \\ d_{n+1,n} &= \mathcal{H}_{n,n} - \frac{n}{n+1}\mathcal{H}_{n,n-1} = -\frac{1}{(n+1)(n+2)} - \frac{n}{n+1} = -\frac{n+1}{n+2}, \\ d_{n+1,k} &= \mathcal{H}_{k,n} - \frac{n}{n+1}\mathcal{H}_{k,n-1} = -\frac{1}{(k+2)(n+1)} + \frac{n}{n+1}\cdot\frac{1}{(k+2)n} = 0 \end{aligned}$$

for $k = 0, 1, \ldots, n-1$.

Our second example is the so-called Rogers–Szegő polynomials (Simon 2005). These polynomials are orthogonal on the unit circle with respect to the measure

$$\mathrm{d}\mu(\theta) = \left[2\pi \log\left(\frac{1}{q}\right)\right]^{-1/2} \sum_{j=-\infty}^{\infty} q^{-(\theta-2\pi)^2/2}\,\mathrm{d}\theta, \qquad q \in (0,1).$$

The monic Rogers–Szegő polynomial has the explicit form

$$\phi_n(z) = \sum_{j=0}^{n} \frac{(-1)^{n-j}(q,q)_n}{(q,q)_j(q,q)_{n-j}} q^{\frac{1}{2}(n-j)} z^j, \tag{3.8}$$

where $(w,q)_n = \prod_{j=0}^{n-1}(1-wq^j)$ is the *q-factorial symbol* (Gasper & Rahman 2004). The corresponding sequence of Schur parameters is given by

$$a_n = (-1)^n q^{n/2}, \qquad n \in \mathbb{Z}_+,$$

and

$$\kappa_n^{-2} = \prod_{j=1}^{n}\left(1-|a_j|^2\right) = \prod_{j=1}^{n}\left(1-q^j\right) = (q,q)_n.$$

Note that the a_ns are real and $-a_{n+1}/a_n \equiv q^{1/2}$. The explicit form of $\mathcal{H}$ follows from Theorem 3: after fairly elementary manipulation, (3.7) yields

$$\mathcal{H}_{k,l} = \begin{cases} (-1)^{k+l} q^{\frac{1}{2}(k+l+1)} \dfrac{(q,q)_l}{(q,q)_k}, & k \le l, \\ 1, & k = l+1, \\ 0, & k \ge l+2. \end{cases}$$

We can in fact do better by direct manipulation of Rogers–Szegő polynomials: Like in Subsection 3.1, we can derive the explicit form of the coefficients $d_{n,m}$ from the expression for the ϕ_ns, i.e. (3.8).

Lemma 4 *For every $n \in \mathbb{Z}_+$ it is true that*

$$z^n = \sum_{m=0}^{n} q^{\frac{1}{2}(n-m)^2} \frac{(q,q)_n}{(q,q)_m(q,q)_{n-m}} \phi_m(z). \tag{3.9}$$

Proof We substitute (3.8) on the right-hand side of (3.9),

$$\begin{aligned}
&\sum_{m=0}^{n} q^{\frac{1}{2}(n-m)^2} \frac{(q,q)_n}{(q,q)_m(q,q)_{n-m}} \sum_{j=0}^{m} \frac{(-1)^{m-j}(q,q)_m}{(q,q)_j(q,q)_{m-j}} q^{\frac{1}{2}(m-j)} z^j \\
&= \sum_{j=0}^{n} \frac{(q,q)_n}{(q,q)_j(q,q)_{n-j}} z^j \sum_{m=j}^{n} (-1)^{m-j} q^{\frac{1}{2}[(n-m)^2+m-j]} \frac{(q,q)_{n-j}}{(q,q)_{n-m}(q,q)_{m-j}} \\
&= \sum_{j=0}^{n} \frac{(q,q)_n}{(q,q)_j(q,q)_{n-j}} q^{\frac{1}{2}(n-j)} z^j \sum_{m=0}^{n-j} (-1)^m q^{\frac{1}{2}[(n-j-m)^2+m]} \frac{(q,q)_{n-j}}{(q,q)_m(q,q)_{n-j-m}}.
\end{aligned}$$

Consequently, it is sufficient to prove that

$$\sum_{m=0}^{N}(-1)^m q^{\frac{1}{2}[(N-m)^2+m]}\frac{(q,q)_N}{(q,q)_m(q,q)_{N-m}} = \begin{cases} 1, & N=0, \\ 0, & N\in\mathbb{N}. \end{cases} \tag{3.10}$$

It is easy to verify that

$$\frac{(q,q)_N}{(q,q)_{N-m}} = (-1)^m q^{\frac{1}{2}(2mN-m^2+m)}(q^{-N},q)_m, \qquad N\in\mathbb{Z}_+,$$

therefore the left-hand side of (3.10) is

$$q^{\frac{1}{2}N^2}\sum_{m=0}^{N}\frac{(q^{-N},q)_m}{(q,q)_m}q^m = q^{\frac{1}{2}(N-1)N}{}_1\phi_0(q^{-N};—;q,q),$$

where

$${}_1\phi_0(a;—;q,z) = \sum_{m=0}^{\infty}\frac{(a,q)_m}{(q,q)_m}z^m$$

is a $(1,0)$ *q-hypergeometric function.* Such function can be represented as a quotient of infinite products,

$${}_1\phi_0(a;—;q,z) = \frac{(az,q)_\infty}{(z,q)_\infty}, \qquad |z|,|q|<1$$

(Gasper & Rahman 2004, p. 7). The substitution $a=q^{-N}$, $z=q$ confirms that (3.10) is true, thereby completing the proof. □

3.3 Expansion coefficients through the Cauchy Integral Theorem

Let

$$f(z) = \sum_{n=0}^{\infty} f_n z^n$$

be an analytic function in an open complex domain Ω which contains the closed unit disc as a subset. Analogously to the OPRL case, we can deduce that

$$\hat{f}_m = \frac{\kappa_m^2}{\kappa_0^2}\sum_{n=m}^{\infty} d_{n,m}f_n, \qquad m\in\mathbb{Z}_+.$$

We again use the Cauchy Integral Theorem to argue that

$$\hat{f}_m = \frac{\kappa_m^2}{\kappa_0^2}\frac{1}{2\pi\mathrm{i}}\int_\gamma f(z)\sum_{n=m}^{\infty}\frac{d_{n,m}}{z^{n+1}}\,\mathrm{d}z,$$

where γ is a simple Jordan-recifiable curve enclosing the the unit disc within Ω.

As in Section 3, we substitute $d_{n,m} = \boldsymbol{e}_m^\top \mathcal{H}^n \boldsymbol{e}_0$ into the formula, whereby

$$\sum_{n=m}^{\infty} \frac{d_{n,m}}{z^{n+1}} = \frac{1}{z} \boldsymbol{e}_m^\top \left(\sum_{n=m}^{\infty} \mathcal{H}^n z^{-n} \right) \boldsymbol{e}_0 = \frac{1}{z^{m+1}} \boldsymbol{e}_m^\top \mathcal{H}^m \left(I - z^{-1}\mathcal{H} \right)^{-1} \boldsymbol{e}_0$$

and, for all $m \in \mathbb{Z}_+$,

$$\hat{f}_m = \frac{\kappa_m^2}{\kappa_0^2} \frac{1}{2\pi \mathrm{i}} \int_\gamma \frac{f(z)}{z^{m+1}} \boldsymbol{e}_m^\top \mathcal{H}^m \left(I - z^{-1}\mathcal{H} \right)^{-1} \boldsymbol{e}_0 \, \mathrm{d}z. \tag{3.11}$$

This is completely analogous to the formula (2.6) for OPRL.

4 Orthogonal Laurent polynomials on the unit circle

4.1 Expansion coefficients through derivatives: general theory

The core methodology of Sections 2–3 lends itself to another important case, *Laurent polynomials* orthogonal on the unit circle.

Given a distribution μ on $\mathbb{T}$, the OPUC system with respect to μ is generated by an orthogonalization of the canonical basis $\{z^n\}_{n \geq 0}$ of $\mathbb{P}$. Analogously, applying the Gram–Schmidt procedure to the basis $\{1, z, z^{-1}, z^2, z^{-2}, \dots\}$, we obtain an orthogonal basis $(\varphi_n)_{n \in \mathbb{Z}_+}$ of Λ. In other words,

(i) $\varphi_n \in \Lambda_{-n,n} \setminus \Lambda_{-(n-1),n-1}$

(ii) $\langle \varphi_{2n}, z^k \rangle_\mu = 0$ for $k = -n+1, \cdots, n$ and $\langle \varphi_{2n+1}, z^k \rangle_\mu = 0$ for $k = -n, \dots, n$.

A sequence on Λ satisfying conditions (i) and (ii) is called a *sequence of orthogonal Laurent polynomials (SOLP)* on $\mathbb{T}$ (Bultheel & Cantero 2009, Cantero et al. 2003, Simon 2005). If in addition $\|\varphi_n\|_\mu = 1$ for all n then we say that $\{\varphi_n\}_{n \in \mathbb{Z}}$ is a sequence of *orthonormal* Laurent polynomals (SONLP).

Given a sequence $\{\varphi_n\}_{n \in \mathbb{Z}_+}$, we define

$$p_{2n}(z) = z^n \bar{\varphi}_{2n}(z^{-1}), \quad p_{2n+1}(z) = z^n \varphi_{2n+1}(z), \qquad n \in \mathbb{Z}_+.$$

Note that $\{\varphi_n\}_{n \in \mathbb{Z}_+}$ is a SOLP if and only if $\{p_n\}_{n \in \mathbb{Z}_+}$ is a sequence of OPUC, because

$$\langle p_{2n}, z^k \rangle = \langle z^{n-k}, \varphi_{2n} \rangle \qquad \text{and} \qquad \langle p_{2n+1}, z^k \rangle = \langle \varphi_{2n+1}, z^{k-n} \rangle.$$

Hence, the polynomial p_{2n} is orthogonal to $1, z, \dots, z^{2n-1}$ if and only if the Laurent polynomial φ_{2n} is orthogonal to $z^{-n+1}, \dots, z^n$, while p_{2n+1} is orthogonal to $1, z, \dots, z^{2n}$ if and only if φ_{2n+1} is orthogonal to $z^{-n}, \dots, z^n$. This establishes a one-to-one correspondence between SOLP (SONLP) and sequences of orthonormal OPUCs. Moreover, the sequence $\{\varphi_n\}_{n \in \mathbb{Z}_+}$ can be obtained from the underlying OPUC using the formulæ

$$\varphi_{2n}(z) = z^{-n} p_{2n}^*(z), \quad \varphi_{2n+1}(z) = z^{-n} p_{2n+1}(z), \qquad n \in \mathbb{Z}_+.$$

We will denote by χ_n the nth orthonormal Laurent polynomial generated in this way by the orthonormal OPUC: it is convenient in the Laurent polynomials' case to normalise in his manner, rather than considering monic polynomials, since it makes for somewhat simpler notation. A fundamental fact about SOLNP is the the χ_ns obey the five-term recurrence relation

$$z\chi_{2n-1} = \rho_{2n}\rho_{2n+1}\chi_{2n+1} - \rho_{2n}a_{2n+1}\chi_{2n} - \bar{a}_{2n-1}a_{2n}\chi_{2n-1} - \rho_{2n-1}a_{2n}\chi_{2n-2}, \quad (4.1)$$
$$z\chi_{2n} = \bar{a}_{2n}\rho_{2n+1}\chi_{2n+1} - \bar{a}_{2n}a_{2n+1}\chi_{2n} + \bar{a}_{2n-1}\rho_{2n}\chi_{2n-1} + \rho_{2n-1}\rho_{2n}\chi_{2n-2} \quad (4.2)$$

(Cantero et al. 2003), where we recall that $\rho_n = (1-|a_n|^2)^{1/2}$, $n \in \mathbb{Z}_+$.

Taking $\{\chi\}_{n\in\mathbb{Z}_+}$ as our basis, there necessarily exist coefficients $d_{n,m}$ such that

$$z^n = \sum_{m=0}^{N_n} d_{n,m}\chi_m, \qquad n \in \mathbb{Z},$$

where

$$N_n = \begin{cases} 2n-1, & n \geq 1, \\ -2n, & n \leq 0. \end{cases}$$

They can be obtained in a standard manner from

$$\langle z^n, \chi_l\rangle = \sum_{m=0}^{N_n} d_{n,m}\langle \chi_m, \chi_l\rangle, \qquad n, l \in \mathbb{Z}.$$

In particular, allowing the two five-term formulæ (4.1–2) play the same role as the three-term recurrence relations in Sections 2 and 3, we obtain the recurrences

$$\begin{aligned} d_{n,2m-1} &= \rho_{2m}\rho_{2m+1}d_{n+1,2m+1} - \rho_{2m}\bar{a}_{2m+1}d_{n+1,2m} - a_{2m-1}\bar{a}_{2m}d_{n+1,2m-1} \\ &\quad - \rho_{2m-1}\bar{a}_{2m}d_{n+1,2m-2}, \\ d_{n,2m} &= a_{2m}\rho_{2m+1}d_{n+1,2m+1} - a_{2m}\bar{a}_{2m+1}d_{n+1,2m} + a_{2m-1}\rho_{2m}d_{n+1,2m-1} \\ &\quad + \rho_{2m-1}\rho_{2m}d_{n+1,2m-2}. \end{aligned}$$

They can be expressed in a matrix form, $\mathcal{C}\boldsymbol{d}_{n+1} = \boldsymbol{d}_n$, hence

$$\boldsymbol{d}_n = \mathcal{C}^{-n}\boldsymbol{e}_0, \qquad n \in \mathbb{Z}, \quad (4.3)$$

where, as before, $\boldsymbol{d}_0 = \boldsymbol{e}_0$, $\boldsymbol{d}_n$ being the column vector $[d_{n,0}, d_{n,1}, d_{n,2}, \cdots]^\top$, $d_{n,m} = 0$, $m \geq n+1$, while

$$\mathcal{C} = \begin{bmatrix} -\bar{a}_1 & \rho_1 & 0 & & & & \\ -\rho_1\bar{a}_2 & -a_1\bar{a}_2 & -\rho_2\bar{a}_3 & \rho_2\rho_3 & & & \\ \rho_1\rho_2 & a_1\rho_2 & -a_2\bar{a}_3 & a_2\rho_3 & 0 & & \\ & 0 & -\rho_3\bar{a}_4 & -a_3\bar{a}_4 & -\rho_4\bar{a}_5 & \rho_4\rho_5 & \\ & & \rho_3\rho_4 & a_3\rho_4 & -a_4\bar{a}_5 & a_4\rho_5 & 0 \\ & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

is the so-called *CMV matrix* (Cantero et al. 2003, Simon 2005) (see also (Watkins 1993)). Once we have the expression (4.3), it is trivial to use the Cauchy Integral Theorem like in Subsection 3.3, expressing the mth expansion coefficient in the SOLP $\{\chi_n\}_{n\in\mathbb{Z}_+}$ similarly to (3.11).

Note that the CMV matrix is always unitary (Cantero, Moral & Velázquez 2005), therefore it is nonsingular and (4.3) can be rewritten in the form

$$\boldsymbol{d}_n = \mathcal{C}^{*n}\boldsymbol{e}_0, \quad \boldsymbol{d}_{-n} = \mathcal{C}^n\boldsymbol{e}_0, \qquad n \in \mathbb{Z}_+.$$

Therefore, given any function f, analytic in an open domain Ω_+ such that $\{z \in \mathbb{Z} : |z| \leq 1\} \subset \Omega_+$, its expansion coefficients in the SOLP basis $\{\chi_n\}_{n\in\mathbb{Z}_+}$ are

$$\hat{f}_n = \frac{1}{2\pi\mathrm{i}} \int_\gamma \frac{f(z)}{z^{n+1}} \boldsymbol{e}_n^\top \mathcal{C}^{*n}(I - z^{-1}\mathcal{C}^*)^{-1}\boldsymbol{e}_0 \,\mathrm{d}z, \qquad n \in \mathbb{Z}_+, \tag{4.4}$$

where γ encircles the unit circle within Ω_+ with winding number 1. Likewise, suppose that f is analytic in an open domain Ω_- such that $\{z \in \mathbb{C} : |z| \geq 1\} \subset \Omega_-$, hence can be expanded into Taylor series in z^{-1}. In that case

$$\hat{f}_n = \frac{1}{2\pi\mathrm{i}} \int_\gamma \frac{f(z)}{z^{n+1}} \boldsymbol{e}_n^\top \mathcal{C}^{n}(I - z^{-1}\mathcal{C})^{-1}\boldsymbol{e}_0 \,\mathrm{d}z, \qquad n \in \mathbb{Z}_+, \tag{4.5}$$

where now γ encircles $\mathbb{T}$ from within with winding number -1. Because of the orthogonality of $\mathcal{C}$, its spectrum lives on the unit circle, therefore in both cases its resolvent – hence the integral – is analytic along γ.

Needless to say, any function f analytic in an open annulus containing T can be written as $f = f_+ + f_-$, where each $f_\pm$ is analytic in some $\Omega_\pm$. In that case we use both (4.4) and (4.5) to expand f in the SONLP system.

4.2 Two examples

Consider the sequence (ϕ_n) of orthogonal polynomials with respect to the Lebesgue measure: trivially, $\phi_n(z) = z^n$, $a_n \equiv 0$, $n \in \mathbb{N}$. Note that $\rho_n \equiv 1$ for all $n \in \mathbb{Z}_+$. The corresponding sequence of Laurent polynomials is

$$\chi_{2n}(z) = z^{-n}, \qquad \chi_{2n+1}(z) = z^{n+1}, \tag{4.6}$$

while the CMV matrix is

$$\mathcal{C} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 1 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 1 & \cdots \\ 0 & 0 & 1 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

By inspection, $\mathcal{C}\boldsymbol{d}_1 = \boldsymbol{e}_0$ is satisfied by $\boldsymbol{d}_1 = \boldsymbol{e}_1$, the second column of $\mathcal{C}$. Likewise, $\mathcal{C}\boldsymbol{d}_2 = \boldsymbol{d}_1 = \boldsymbol{e}_1$ is satisfied by the fourth column of $\mathcal{C}$, therefore $\boldsymbol{d}_2 = \boldsymbol{e}_3$. Likewise, $\boldsymbol{d}_3 = \boldsymbol{e}_5$ and, in general, it is easy to prove by induction that $\boldsymbol{d}_n = \boldsymbol{e}_{2n-1}$ for $n \in \mathbb{N}$, consistently with (4.6).

A more careful examination of $\mathcal{C}$ reveals an interesting state of affairs. Clearly, each section of this matrix has either bottom row or rightmost column of zeros, hence is singular.Of course, this is not the case with the infinite-dimensional unitary matrix!

In our second example we return to the Rogers–Szegő polynomials, except that now we consider them in the SONLP setting. Recall that $a_n = (-1)^n q^{n/2}$ and $\rho_n = (1-q^n)^{1/2}$. Normalizing (3.8) to render them monic yields

$$p_n(z) = \frac{1}{(q,q)_n^{1/2}} \sum_{j=0}^{n} \frac{(-1)^{n-j}(q,q)_n}{(q,q)_j(q,q)_{n-j}} q^{\frac{1}{2}(n-j)} z^j,$$

therefore

$$\chi_{2n}(z) = z^{-n} p_{2n}^*(z) = \frac{1}{(q,q)_{2n}^{1/2}} \sum_{j=0}^{2n} \frac{(-1)^j (q,q)_{2n}}{(q,q)_j(q,q)_{2n-j}} q^{n-\frac{1}{2}j} z^{n-j},$$

$$\chi_{2n+1}(z) = z^{-n} p_{2n+1}(z) = -\frac{1}{(q,q)_{2n+1}^{1/2}} \sum_{j=0}^{2n+1} \frac{(-1)^j (q,q)_{2n+1}}{(q,q)_j(q,q)_{2n+1-j}} q^{n-\frac{1}{2}(j-1)} z^{j-n}.$$

Lemma 5 *For Rogers–Szegő SONLP we have*

$$d_{n,m} = q^{\alpha_{n,m}/2}(q,q)_m^{1/2} \frac{(q,q)_{n+\lfloor (m-1)/2 \rfloor}}{(q,q)_m (q,q)_{n-\lfloor m/2 \rfloor -1}}, \qquad n \in \mathbb{Z}_+, \tag{4.7}$$

$$d_{-n,m} = (-1)^m q^{\beta_{n,m}/2}(q,q)_m^{1/2} \frac{(q,q)_{n+\lfloor m/2 \rfloor}}{(q,q)_m (q,q)_{n-\lfloor (m+1)/2 \rfloor}}, \qquad n \in \mathbb{N}, \tag{4.8}$$

where

$$\alpha_{n,m} = (n - \lfloor (m+1)/2 \rfloor)^2 + \begin{cases} m, & m \text{ even}, \\ 0, & \text{odd}, \end{cases}$$

$$\beta_{n,m} = (n - \lfloor m/2 \rfloor)^2 + \begin{cases} 0, & m \text{ even}, \\ m, & m \text{ odd}. \end{cases}$$

Proof We commence by listing all the nonzero terms of the CMV matrix: for all relevant values of $m \in \mathbb{Z}_+$

$$\begin{aligned} \mathcal{C}_{2m,2m-2} &= \rho_{2m-1}\rho_{2m}, & \mathcal{C}_{2m,2m-1} &= a_{2m-1}\rho_{2m}, \\ \mathcal{C}_{2m,2m} &= -a_{2m}\bar{a}_{2m+1}, & \mathcal{C}_{2m,2m+1} &= a_{2m}\rho_{2m+1}, \\ \mathcal{C}_{2m+1,2m} &= -\rho_{2m+1}\bar{a}_{2m+2}, & \mathcal{C}_{2m+1,2m+1} &= -a_{2m+1}\bar{a}_{2m+2}, \\ \mathcal{C}_{2m+1,2m+2} &= -\rho_{2m+2}\bar{a}_{2m+3}, & \mathcal{C}_{2m+1,2m+3} &= \rho_{2m+2}\rho_{2m+3}. \end{aligned}$$

For simplicity we prove (4.7) just for even ms – the proof for odd values of m is identical. The statement is true for $n = 0$ and we continue by induction on n. Using the relation $\boldsymbol{d}_{n+1} = \mathcal{C}^* \boldsymbol{d}_n$, we have

$$\begin{aligned}
d_{n+1,2m} &= \sum_{k=0}^{\infty} \mathcal{C}_{k,2m} d_{n,k} \\
&= q^{2m+\frac{1}{2}} d_{n,2m} - q^{m+1}(1-q^{2m+1})^{1/2} d_{n,2m+1} + q^{m+\frac{1}{2}}(1-q^{2m})^{1/2} d_{n,2m-1} \\
&\quad + (1-q^{2m+1})^{1/2}(1-q^{2m+2})^{1/2} d_{n,2m+2} \\
&= q^{2m+\frac{1}{2}+\frac{1}{2}\alpha_{n,2m}} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m-1}}{(q,q)_{2m}(q,q)_{n-m-1}} \\
&\quad - q^{m+1+\frac{1}{2}\alpha_{n,2m+1}} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m}}{(q,q)_{2m}(q,q)_{n-m-1}} \\
&\quad + q^{m+\frac{1}{2}+\frac{1}{2}\alpha_{n,2m-1}} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m-1}}{(q,q)_{2m}(q,q)_{n-m}} \\
&\quad + q^{\frac{1}{2}\alpha_{n,2m+2}} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m}}{(q,q)_{2m}(q,q)_{n-m-2}} \\
&= q^{\frac{1}{2}[(n-m)^2+1]} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m-1}}{(q,q)_{2m}(q,q)_{n-m}} \left[q^{3m}(1-q^{n-m}) \right. \\
&\qquad - q^{2m-n+1}(1-q^{n-m})(1-q^{n+m}) + q^m(1-q^{2m}) \\
&\qquad \left. + q^{2m-n+1}(1-q^{n-m-1})(1-q^{n-m})(1-q^{n+m}) \right].
\end{aligned}$$

But

$$q^{3m}(1-q^{n-m}) + q^m(1-q^{2m}) = q^m(1-q^{n+m}),$$

therefore

$$\begin{aligned}
d_{n+1,2m} &= q^{\frac{1}{2}[(n-m)^2+m+11]} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m}}{(q,q)_{2m}(q,q)_{n-m}} \\
&\qquad \times \left\{ 1 - q^{m-n+1}(1-q^{n-m}) \left[1 - (1-q^{n-m-1}) \right] \right\} \\
&= q^{\alpha_{n+1,2m}/2} (q,q)_{2m}^{1/2} \frac{(q,q)_{n+m}}{(q,q)_{2m}(q,q)_{n-m}},
\end{aligned}$$

consistently with (4.7).

We turn our attention to (4.8). Now, for variety sake, we prove it for odd values of m. The argument is again inductive, based upon the recursion $\boldsymbol{d}_{-n-1} = \mathcal{C} \boldsymbol{d}_{-n}$,

$n \in \mathbb{Z}_+$. Given the quindiagonal structure of $\mathcal{C}$, we have

$$\begin{aligned}
d_{-n-1,2m+1} &= \mathcal{C}_{2m+1,2m} d_{-n,2m} + \mathcal{C}_{2m+1,2m+1} d_{-n,2m+1} + \mathcal{C}_{2m+1,2m+2} d_{-n,2m+2} \\
&\quad + \mathcal{C}_{2m+1,2m+3} d_{-n,2m+3} \\
&= -q^{\frac{1}{2}(n-m)^2+m+1} (q,q)_{2m+1}^{1/2} \frac{(q,q)_{n+m}}{(q,q)_{2m}(q,q)_{n-m}} \\
&\quad - q^{\frac{1}{2}(n-m)^2+3m+2} (q,q)_{2m+1}^{1/2} \frac{(q,q)_{n+m}}{(q,q)_{2m+1}(q,q)_{n-m-1}} \\
&\quad + q^{\frac{1}{2}(n-m)^2-n+2m+2} (q,q)_{2m+1}^{1/2} \frac{(q,q)_{n+m+1}}{(q,q)_{2m+1}(q,q)_{n-m-1}} \\
&\quad - q^{\frac{1}{2}(n-m)^2-n+2m+2} (q,q)_{2m+1}^{1/2} \frac{(q,q)_{n+m+1}}{(q,q)_{2m+1}(q,q)_{n-m-2}} \\
&= q^{\frac{1}{2}(n-m)^2} (q,q)_{2m+1}^{\frac{1}{2}} \frac{(q,q)_{n+m}}{(q,q)_{2m+1}(q,q)_{n-m}} \left[-q^{m+1}(1-q^{2m+1}) \right. \\
&\qquad - q^{3m+2}(1-q^{n-m}) + q^{-n+2m+2}(1-q^{n+m+1})(1-q^{n-m}) \\
&\qquad \left. - q^{-n+2m+2}(1-q^{n+m+1})(1-q^{n-m-1})(1-q^{n-m}) \right] \\
&= -q^{\frac{1}{2}[(n+1-m)^2+2m+1]} (q,q)_{2m+1}^{1/2} \frac{(q,q)_{n+m+1}}{(q,q)_{2m+1}(q,q)_{n-m}},
\end{aligned}$$

as claimed by (4.8). This concludes the proof. □

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