Sobolev-Orthogonal Systems with Tridiagonal Skew-Hermitian Differentiation Matrices

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Abstract

We introduce and develop a theory of orthogonality with respect to Sobolev inner products on the real line for sequences of functions with a tridiagonal, skew-Hermitian differentiation matrix. While a theory of such L_2-orthogonal systems is well established, Sobolev orthogonality requires new concepts and their analysis. We characterise such systems completely as appropriately weighted Fourier transforms of orthogonal polynomials and present a number of illustrative examples, inclusive of a Sobolev-orthogonal system whose leading N coefficients can be computed in $\mathcal{O}(N \log N)$ operations.

Keywords Orthogonal systems, Sobolev orthogonality, spectral methods, Malmquist–Takenaka functions
Mathematics Subject Classification 42C05, 42C10, 42C30, 65M12, 65M70

1 Introduction

1.1 Orthonormal systems on the real line

The theory of L_2-orthonormal systems on the real line with a tridiagonal differentiation matrix has been developed in (Iserles & Webb 2019, Iserles & Webb 2020, Iserles & Webb 2021*b*, Iserles & Webb 2021*a*). In its simplest (real) version, let $w \geq 0$ be an absolutely continuous, nonzero weight function, whose support is symmetric with respect to the origin, and $\{p_n\}_{n\in\mathbb{Z}_+}$ the underlying system of orthonormal polynomials, which must satisfy

$$b_n p_{n+1}(\xi) = \xi p_n(\xi) - b_{n-1} p_{n-1}(\xi), \qquad n \in \mathbb{Z}_+.$$

for some real numbers $\{b_n\}_{n\in\mathbb{Z}_+}$. Setting

$$\varphi_n(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p_n(\xi)\sqrt{w(\xi)}\mathrm{e}^{\mathrm{i}x\xi}\,\mathrm{d}\xi, \qquad x \in \mathbb{R}, \quad n \in \mathbb{Z}_+, \tag{1.1}$$

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we obtain by Parseval's theorem[1] an orthonormal system of functions in $L_2(\mathbb{R})$. Moreover, under the mild assumption that polynomials are dense in $L_2(\mathbb{R}; w)$, this system is dense in $L_2(\mathbb{R})$ if the support of w is all of $\mathbb{R}$, otherwise its closure is the *Paley–Wiener space* $\mathcal{PW}_{\operatorname{supp} w}(\mathbb{R})$ of all $L_2(\mathbb{R})$ functions whose Fourier transform is supported on $\operatorname{supp} w$. Moreover, $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+}$ obeys

$$\varphi_n'(x) = -b_{n-1}\varphi_{n-1}(x) + b_n\varphi_{n+1}(x), \qquad n \in \mathbb{Z}_+. \tag{1.2}$$

In vector form, (1.2) is $\boldsymbol{\varphi}' = \mathcal{D}\boldsymbol{\varphi}$, where $\mathcal{D}$ is the *differentiation matrix* of the system, which in this case is tridiagonal and skew-symmetric. Skew symmetry and the tridiagonal form provide important advantages on the design of spectral methods with the basis Φ (Iserles & Webb 2019).

In this paper we generalise the theory to the case of Sobolev-orthogonal systems, where the Sobolev inner product is of the form

$$\langle \varphi, \psi\rangle_v = \sum_{\ell=0}^{\infty} v_\ell \int_{-\infty}^{\infty} \varphi^{(\ell)}(x)\overline{\psi^{(\ell)}(x)}\,\mathrm{d}x,$$

defined by the non-zero, non-negative sequence $\{v_\ell\}_{\ell\in\mathbb{Z}_+} \subset [0,\infty)$. The $\mathbf{H}_2^s(\mathbb{R})$ norm, where $s \in \mathbb{Z}_+$ corresponds to $v_\ell = 1$ for $\ell = 0, 1 \ldots, s$ and $v_\ell = 0$ otherwise.

Besides the resulting theory being of interest in its own right, we can motivate our exploration in the context of spectral methods for PDEs using the example of the Ornstein–Uhlenbeck process,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - a\frac{\partial}{\partial x}(xu), \qquad x \in \mathbb{R}, \quad t \geq 0, \tag{1.3}$$

with coefficient of friction described by the positive constant a (Da Prato & Zabczyk 2014, Lawler 2006). Solutions to this PDE satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} [u_x^2(x) + u^2(x)]\,\mathrm{d}x = -\int_{-\infty}^{\infty} [2u_{xx}^2(x) + (2+3a)\,u_x^2(x) + au^2(x)]\,\mathrm{d}x, \tag{1.4}$$

which shows that the solution decays monotonically to zero in the $\mathbf{H}_2^1(\mathbb{R})$ norm. In fact, we can drop some terms and show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle u, u\rangle_{H^1} \leq -a\langle u, u\rangle_{H^1}$, and hence the norm decreases at least exponentially with rate dependent on a.

Now, consider semi-discretising equation (1.3) in space by a spectral method $u(x,t) \approx u_N(x,t) := \sum_{n=0}^{N} a_n(t)\varphi_n(x)$, where $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+} \subset L_2(\mathbb{R})$ are orthonormal with respect to the $\mathbf{H}_2^1(\mathbb{R})$ inner product. If a Galerkin scheme is used with respect to the $\mathbf{H}_2^1(\mathbb{R})$ inner product (i.e. the residual of the PDE at each time t is orthogonal to $\operatorname{span}\{\varphi_n\}_{n=0}^{N}$), then the inequality (1.4) is also satisfied by u_N (cf. (Hesthaven, Gottlieb & Gottlieb 2007, Ch. 8)). It therefore follows that any A-stable discretisation in time will be stable.

The plan of this paper is as follows. In Section 2, basing ourselves upon our earlier theory on L_2 inner products, we present a complete framework for the construction of Sobolev-orthogonal systems on the real line with a tridiagonal differentiation matrix.

[1] Also known as Plancharel's theorem.

This leads to two alternatives towards the construction of $\mathbf{H}_2^s(\mathbb{R})$-orthogonal systems, which are debated in Section 3: the first is the arguably more obvious approach, yet it leads to formulæ which typically are impossible to express explicitly, while the second, less natural, results in a more constructive approach. Section 4 is concerned with systems based upon the familiar Hermite weight and Section 5 with bilateral (i.e., symmetrised with respect to the origin) Laguerre weights. In Section 6 we discuss Bessel-like orthogonal systems originating in various ultraspherical weights: in that case the closure of the orthogonal system is not $\mathbf{H}_2^s(\mathbb{R})$ but a relevant Paley–Wiener space. Section 7 generalises the discourse to non-symmetric measures. In that instance our orthogonal systems are complex-valued but the approach confers some important advantages. In particular, it allows us to generalise the Malmquist–Takenaka system to Sobolev setting while retaining the most welcome feature of this system, namely that the coefficients can be computed rapidly with Fast Fourier Transform. Finally, in Section 8 we present brief conclusions.

1.2 Sobolev norms beyond this paper

As an aside, our original interest in orthonormal systems (1.1) has been motivated in (Iserles & Webb 2019) by the numerical solution of the linear Schrödinger equation in the semi-classical regime,

$$\mathrm{i}\varepsilon\frac{\partial u}{\partial t} = -\varepsilon^2\frac{\partial^2 u}{\partial x^2} + V(x)u, \qquad x\in\mathbb{R}, \quad t\geq 0,$$

given with an initial condition at $t=0, x\in\mathbb{R}$. Here $0<\varepsilon\ll 1$, while the *interaction potential* V is real. The solution of this equation conserves the standard L_2 norm (which motivates the use of L_2-orthogonal systems), but it also has another important invariant: its Hamiltonian,

$$H(u) = \int_{-\infty}^{\infty} [\varepsilon|u_x(x)|^2 + \varepsilon^{-1}V(x)|u(x)|^2]\,\mathrm{d}x,$$

is conserved. This might be viewed as a conservation of a non-standard Sobolev norm (if V is positive). While the design of Hamiltonian methods for the Schrödinger equation is still an open problem, it motivates the work reported in this paper.

We mention in passing another example in which nonstandard Sobolev norms are non-increasing, the diffusion equation,

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[a(x)\frac{\partial u}{\partial x}\right], \qquad x\in\mathbb{R}, \quad t\geq 0,$$

where $a(x)>a_{\min}>0$ for all $x\in\mathbb{R}$, given with an initial condition for $t=0, x\in\mathbb{R}$. It is readily shown that the norm induced by the following nonstandard Sobolev inner product is non-increasing as a function of time,

$$\langle u,u\rangle_a := \int_{-\infty}^{\infty}[a(x)u_x^2(x)+u^2(x)]\,\mathrm{d}x.$$

We do not pursue these general Sobolev inner products in this paper, but anticipate reporting on such results in the future.

1.3 Related work

Sobolev orthogonality: Polynomials orthogonal with respect to Sobolev inner products associated with a vector of measures supported on the real line have been considered for a long while but the subject received considerable impetus with the introduction of coherent pairs in (Iserles, Koch, Nørsett & Sanz-Serna 1991) and has been surveyed in (Marcellán, Alfaro & Rezola 1993, Marcellán & Xu 2015). Natural questions, given the constructs (1.1) and (1.2) are, firstly, how to generate Sobolev-orthogonal systems on the real line and, secondly, is a Fourier integral of an orthogonal polynomial system scaled by *any* reasonable function orthogonal with respect to *some* inner product, whether in a classical or Sobolev sense, in line with the L_2 theory as briefly reviewed in Section 2. These related questions are the focus of this paper. Intriguingly, as things stand, the theory in this paper is heavily based on the theory of classical orthogonal polynomials (as distinct from Sobolev-orthogonal polynomials).

Fourier–Bessel functions (Diekema & Koornwinder 2012, Mantica 2006): Given a Borel measure $\mathrm{d}\mu$ and the underlying orthonormal system $\{p_n\}_{n\in\mathbb{Z}_+}$, we define

$$\varphi_n(x) = \int_{-\infty}^{\infty} p_n(\xi)\mathrm{e}^{-\mathrm{i}x\xi}\,\mathrm{d}\mu(\xi) \tag{1.5}$$

as the nth *Fourier–Bessel function:* the name is motivated by the Legendre measure $\mathrm{d}\mu(x) = \chi_{(-1,1)}(x)\,\mathrm{d}x$, whereby $\varphi_n(x) = \sqrt{2\pi/x}\mathrm{J}_{n+\frac{1}{2}}(x)$. Note the similarity between (1.1) and (1.5) (disregarding the normalising factor and the sign in the exponential, neither of which is of much importance), namely that both are Fourier transforms of p_n with added scaling function: $\sqrt{w}$ in the first instance, w in the second.

Further variation on this theme is the identity

$$\int_{-1}^{1} \mathrm{T}_n(\xi)\mathrm{e}^{\mathrm{i}x\xi}\frac{\mathrm{d}\xi}{\sqrt{1-\xi^2}} = \pi\mathrm{i}^n\mathrm{J}_n(x), \qquad n\in\mathbb{Z}_+, \tag{1.6}$$

where T_n is the nth Chebyshev polynomial of the first kind (Diekema & Koornwinder 2012). Note that, unlike (1.1), Fourier–Bessel functions need not be orthogonal although, interestingly enough, disregarding signs and normalising constants, the two formulæ coincide (and orthogonality is recovered) for the Legendre measure.

1.4 Brief comments

The name of Charles Hermite is associated with two distinct concepts in this paper: skew-Hermitian matrices and Hermite polynomials. They are of course completely different and should not be confused.

Our notation deserves a comment. Thus, we let $\mathbf{H}_2^s$, where $s \geq 0$, stand for the usual Sobolev space, equipped with the inner product

$$\langle f, g\rangle = \sum_{k=0}^{s} v_k \int f^{(k)}(\xi) g^{(k)}(x)\,\mathrm{d}x,$$

where the v_ks are nonnegative and $v_0 > 0$. With greater generality, it is often helpful to denote

$$\mathbf{H}_{2,v}(\mathbb{R}) := \{\psi \in \mathrm{L}_2(\mathbb{R}) : \langle\psi,\psi\rangle_v < \infty\}, \tag{1.7}$$

whenever $\langle \cdot, \cdot \rangle_v$ is an inner product defined (in a sense which is always clear from the context) by a function v.

2 Characterisation of Sobolev-orthogonal systems

Let us first state the desiderata. We are interested in functions $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+} \subset \mathrm{L}_2(\mathbb{R})$ such that *both* of the following properties hold.

(A) There exists sequences $\{b_n\}_{n\in\mathbb{Z}_+} \subset \mathbb{C} \setminus \{0\}$ and $\{c_n\}_{n\in\mathbb{Z}_+} \subset \mathbb{R}$ such that

$$\varphi_n'(x) = -\overline{b_{n-1}}\varphi_{n-1}(x) + \mathrm{i}c_n\varphi_n(x) + b_n\varphi_{n+1}(x) \tag{2.1}$$

for $n = 0, 1, \ldots$ (with $b_{-1} = 0$ by convention);

(B) Φ is an orthonormal sequence with respect to the Sobolev inner product

$$\langle \varphi, \psi \rangle_v = \sum_{\ell=0}^{\infty} v_\ell \int_{-\infty}^{\infty} \varphi^{(\ell)}(x)\overline{\psi^{(\ell)}(x)}\,\mathrm{d}x, \tag{2.2}$$

defined by the non-zero, non-negative sequence $\{v_\ell\}_{\ell\in\mathbb{Z}_+} \subset [0,\infty)$ such that $\sum_{\ell=0}^{\infty} v_\ell > 0$. (In other words, at least one v_ℓ must be positive.)

Theorem 1 ((Iserles & Webb 2019, Iserles & Webb 2020)) *A sequence* $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+} \subset \mathrm{L}_2(\mathbb{R})$ *satisfies criterion (A) if and only if*

$$\varphi_n(x) = \frac{\mathrm{e}^{\mathrm{i}\theta_n}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}x\xi} p_n(\xi) g(\xi)\,\mathrm{d}\xi, \tag{2.3}$$

where

- $P = \{p_n\}_{n\in\mathbb{Z}_+}$ *is an orthonormal polynomial system on the real line with respect to a probability measure on the real line with all moments finite and with infinitely many points of increase;*
- $\Theta = \{\theta_n\}_{n\in\mathbb{Z}_+} \subset [0, 2\pi)$*;*
- $g \in \mathrm{L}_2(\mathbb{R})$ *satisfies* $\lim_{\xi\to\pm\infty} |\xi^k g(\xi)| = 0$ *for* $k = 0, 1, 2, \ldots$. *We call such functions* mollifiers.

Remark 2 *It is possible to ensure that the parameters* $\{b_n\}_{n\in\mathbb{Z}_+}$ *satisfy* $b_n > 0$ *without any genuine loss of generality. This is achieved by simply setting* $\mathrm{e}^{\mathrm{i}\theta_n} = \mathrm{i}^n$. *We henceforth assume that* $b_n > 0$.

Remark 3 *Under the assumption of Remark 2, the functions* Φ *are real if and only if* $g(\xi)$ *has even real part and odd imaginary part (with respect to the origin), and* P *is orthonormal with respect to an even measure (with respect to the origin). In this case,* $b_n > 0$ *and* $c_n = 0$ *for all* n.

Theorem 1 and Remarks 2 and 3 were proved by the present authors in (Iserles & Webb 2019, Iserles & Webb 2020) along with results characterising when such systems are orthogonal with respect to the standard inner product on $\mathrm{L}_2(\mathbb{R})$. The following Theorem generalises these orthogonality results to the Sobolev inner products in equation (2.2).

Theorem 4 *Let φ satisfy criterion (A), which implies that* (2.3) *holds. Then φ also satisfies criterion (B) if and only if the mollifier g satisfies*

$$w(\xi) = v(\xi)|g(\xi)|^2, \tag{2.4}$$

where $w(\xi)$ is the positive weight function with respect to which the polynomials P are orthonormal, and $v(\xi) = \sum_{\ell=0}^{\infty} v_\ell \xi^{2\ell}$. In particular, it is necessary for the non-negative sequence $\{v_\ell\}_{\ell\in\mathbb{Z}_+}$ to decay sufficiently fast that $v(\xi)$ is finite on the support of w.

Proof By Parseval's Theorem,

$$\int_{-\infty}^{\infty} \varphi_n(x)\overline{\varphi_m(x)}\,\mathrm{d}x = (-\mathrm{i})^{m-n}\int_{-\infty}^{\infty} p_n(\xi)p_m(\xi)|g(\xi)|^2\,\mathrm{d}\xi.$$

Furthermore, since $\widehat{\varphi^{(\ell)}}(\xi) = (-\mathrm{i}\xi)^\ell\hat{\varphi}(\xi)$ (where $\hat{\varphi}$ denotes the Fourier transform of φ) we have

$$\int_{-\infty}^{\infty} \varphi_n^{(\ell)}(x)\overline{\varphi_m^{(\ell)}(x)}\,\mathrm{d}x = (-\mathrm{i})^{m-n}\int_{-\infty}^{\infty} p_n(\xi)p_m(\xi)\xi^{2\ell}|g(\xi)|^2\,\mathrm{d}\xi.$$

Therefore,

$$\langle\varphi_n,\varphi_m\rangle_v = (-\mathrm{i})^{m-n}\int_{-\infty}^{\infty} p_n(\xi)p_m(\xi)v(\xi)|g(\xi)|^2\,\mathrm{d}\xi$$

This makes it clear that φ is orthonormal with respect to the Sobolev inner product if and only if P is orthonormal with respect to the measure $v(\xi)|g(\xi)|^2\mathrm{d}\xi$. □

Remark 5 *There are infinitely many choices of g which satisfy* (2.4)*, namely*

$$g(\xi) = \sqrt{\frac{w(\xi)}{v(\xi)}}\mathrm{e}^{\mathrm{i}\vartheta(\xi)},$$

for any measurable real-valued function ϑ. Our canonical choice is $\vartheta \equiv 0$, although we know of no good reason, except for simplicity, why this might be superior to other choices.

It is important to answer what space the resulting orthonormal system is dense in: ideally this is the inner product space (1.7), endowed with the inner product $\langle\cdot,\cdot\rangle_v$, but this need not be the case.

Theorem 6 (Orthogonal bases of Paley–Wiener spaces) *Let $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+}$ satisfy the requirements of Theorem 4 with weight function $w(\xi)$ such that polynomials are dense in $\mathrm{L}_2(\mathbb{R}; w(\xi)\mathrm{d}\xi)$. Then Φ forms a basis for the closure (in $\mathbf{H}_{2,v}(\mathbb{R})$) of the Paley–Wiener space $\mathcal{PW}_\Omega(\mathbb{R})$, where Ω is the support of w.*

A proof of Theorem 6 can be obtained by modifying Theorem 9 from (Iserles & Webb 2019). The key corollary is that for a basis Φ satisfying the requirements of Theorem 4 to be complete in $\mathrm{L}_2(\mathbb{R})$, it is necessary that the polynomial basis P is orthogonal with respect to a measure which is supported on the whole real line.

3 Sobolev cascades

In this section we derive two methods for producing orthonormal systems in the Sobolev space $\mathbf{H}_2^s(\mathbb{R})$ where $s = 0, 1, 2, \ldots$.

3.1 Cascades of first and second kind

For a weight function w and $s \in \mathbb{Z}_+$ we can define the following two sequences of bases:

$$\varphi_n^{\langle s \rangle}(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}x\xi}\, p_n(\xi) \sqrt{\frac{w(\xi)}{\sum_{k=0}^{s} \xi^{2k}}}\, \mathrm{d}\xi, \tag{3.1}$$

where $P = \{p_n\}_{n\in\mathbb{Z}_+}$ are orthonormal polynomials with respect to $w(\xi)$, and

$$\varphi_n^{[s]}(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}x\xi}\, p_n^{[s]}(\xi) \sqrt{w(\xi)}\, \mathrm{d}\xi, \tag{3.2}$$

where $P^{[s]} = \{p_n^{[s]}\}_{n\in\mathbb{Z}_+}$ are orthonormal polynomials with respect to the weight

$$w^{[s]}(\xi) = \left(\sum_{k=0}^{s} \xi^{2k}\right) w(\xi) = \frac{1-\xi^{2(s+1)}}{1-\xi^2} w(\xi).$$

By the theory described in Section 2, both systems $\Phi^{\langle s \rangle} = \{\varphi_n^{\langle s \rangle}\}_{n\in\mathbb{Z}_+}$ and $\Phi^{[s]} = \{\varphi_n^{[s]}\}_{n\in\mathbb{Z}_+}$ have skew-Hermitian tridiagonal differentiation matrices and both are orthonormal systems with respect to the standard $\mathbf{H}_2^s(\mathbb{R})$ Sobolev inner product described in the introduction. Furthermore, all of these systems are bases for (closure of) the Paley–Wiener space $\mathcal{PW}_\Omega(\mathbb{R})$, where Ω is the support of w.

We call the sequence $\Phi^{\langle 0 \rangle}, \Phi^{\langle 1 \rangle}, \Phi^{\langle 2 \rangle} \ldots$ a *Sobolev cascade of the first kind* for the weight function w, and $\Phi^{[0]}, \Phi^{[1]}, \Phi^{[2]} \ldots$ a *Sobolev cascade of the second kind* for the weight function w. Note that $\varphi_n^{[0]} = \varphi_n^{\langle 0 \rangle}$.

While a cascade of the first kind is perhaps a more natural generalisation of L_2-orthogonality, it is also more problematic. Typically the polynomials p_n might be already known, however the explicit form of the integrals (3.1), hence of the $\varphi_n^{\langle s \rangle}$s, is often unknown, even for $s = 1$. The issue with cascades of the second kind is different: the polynomials $P^{[s]}$ are usually unknown for $s \in \mathbb{N}$ even for the most familiar measures like Legendre or Hermite. On the other hand, once we know $p_n^{[s]}$ and can compute $\varphi_n^{[0]}$ explicitly, the closed form of $\varphi_n^{[s]}$ is available for all $n, s \in \mathbb{Z}_+$ through the integral (3.2). Note that to compute (1.1) in a closed form we need to be able to integrate explicitly Fourier transforms of $p\sqrt{w}$ for polynomials p: exactly the same is required for the computation of (3.2).

3.2 Sobolev cascades of the second kind

Orthogonal systems in a cascade of the second kind have a simple relationship. The following theorem is a straightforward consequence of the *Geronimus transformation* (Gautschi 2004).

Theorem 7 *Let $s \in \mathbb{Z}_+$. There exists an infinite, lower triangular matrix $C^{[s]}$ which has bandwidth $2s$, such that*

$$\boldsymbol{\varphi}^{[0]} = C^{[s]}\boldsymbol{\varphi}^{[s]}, \tag{3.3}$$

where $\boldsymbol{\varphi}^{[s]}$ are the elements of $\Phi^{[s]}$, arranged into a column vector.

Proof Since $p_n^{[0]}$ and $p_n^{[s]}$ are polynomials of degree n (for every n), there exists a lower triangular *connection coefficient matrix* $\tilde{C}^{[s]}$ such that

$$p_n^{[0]} = \sum_{j=0}^{n} \tilde{C}_{n,j}^{[s]} p_j^{[s]}. \tag{3.4}$$

Since $P^{[s]}$ is an orthonormal basis with respect to the weight function $\left(\sum_{k=0}^{s} \xi^{2k}\right) w(\xi)$, we have the formula

$$\tilde{C}_{n,j}^{[s]} = \int_{-\infty}^{\infty} p_n^{[0]}(\xi) p_j^{[s]}(\xi) \left(\sum_{k=0}^{s} \xi^{2k}\right) w(\xi)\,\mathrm{d}\xi. \tag{3.5}$$

Since $p_j^{[s]}(\xi)\left(\sum_{k=0}^{s} \xi^{2k}\right)$ is a polynomial of degree at most $j+2s$, and $P^{[0]}$ is orthonormal with respect to w, we have that $C_{n,j}^{[s]} = 0$ if $j \le n - 2s - 1$, which proves the desired bandwidth of the matrix. The proof is completed by multiplying equation (3.4) by $\sqrt{w(\xi)}$ and taking the inverse Fourier transform:

$$\varphi_n^{[0]} = \sum_{j=0}^{n} C_{n,j}^{[s]} \varphi_j^{[s]}, \text{ where } C_{n,j}^{[s]} = \mathrm{i}^{n-j} \tilde{C}_{n,j}^{[s]}. \tag{3.6}$$

□

Note further that if the weight function w is symmetric then all the polynomials $p_n^{[s]}$ maintain the parity of n and it follows easily that $C_{n,j}^{[s]} = 0$ for $n + j$ odd.

Theorem 7 has two consequences. Firstly, if one can calculate $\{\varphi_0^{[0]}, \varphi_1^{[0]}, \ldots, \varphi_N^{[0]}\}$, then it is possible to calculate $\{\varphi_0^{[s]}, \varphi_1^{[s]}, \ldots, \varphi_N^{[s]}\}$ in $\mathcal{O}(N)$ operations by applying forward substitution to the banded lower triangular system with matrix $C^{[s]}$.

Secondly, given $N+1$ expansion coefficients in the basis $\Phi^{[0]}$, we can compute the equivalent expansion coefficients in the basis $\Phi^{[s]}$ in $\mathcal{O}(N)$ operations. Specifically, if

$$\sum_{n=0}^{N} a_n^{[0]} \varphi_n^{[0]}(x) = \sum_{n=0}^{N} a_n^{[s]} \varphi_n^{[s]}(x),$$

then

$$C^{[s]\top} \boldsymbol{a}^{[\boldsymbol{s}]} = \boldsymbol{a}^{[\boldsymbol{0}]}, \tag{3.7}$$

which can be solved in $\mathcal{O}(N)$ operations by back substitution.

A neat idea has been suggested by one of the referees. Let $\tilde{C}^{[s]} = LL^\top$ be a Cholesky factorisation of the symmetric matrix $\tilde{C}^{[s]}$ and set

$$\boldsymbol{p}^{[s]}(\xi) = \begin{bmatrix} p_0^{[s]}(\xi) \\ p_1^{[s]}(\xi) \\ p_2^{[s]}(\xi) \\ \vdots \end{bmatrix}.$$

Therefore $\tilde{C}^{[0]} = \langle \boldsymbol{p}^{[0]}, \boldsymbol{p}^{[0]} \rangle_{w_s}$, where $\langle \,\cdot\,, \,\cdot\, \rangle_{w_s}$ is the inner product corresponding to the measure $\prod_{j=1}^{s} \xi^{2j} \,\mathrm{d}\mu(\xi)$.

Orthonormality of the $\{p_n^{[s]}\}_{n\in\mathbb{Z}_+}$ implies that $\langle \boldsymbol{p}^{[s]}, \boldsymbol{p}^{[s]} \rangle_{w_s} =$, while (3.4) means that $\boldsymbol{p}^{[s]} = \tilde{C}^{[s]^{-1}} \boldsymbol{p}^{[0]}$. Therefore

$$I = \tilde{C}^{[s]^{-1}} \langle \boldsymbol{p}^{[0]}, \boldsymbol{p}^{[0]} \rangle_{w_s} \tilde{C}^{[s]^{-\top}} = \tilde{C}^{[s]^{-1}} LL^\top \tilde{C}^{[s]^{-\top}} = (\tilde{C}^{[s]^{-1}} L)(\tilde{C}^{[s]^{-1}} L)^\top.$$

We deduce that $\tilde{C}^{[s]^{-1}} L$ is an idempotent matrix and, both $\tilde{C}^{[s]}$ and L being lower triangular, deduce that $\tilde{C}^{[s]} = L$. Therefore, practical calculation of connection coefficients involves just Cholesky factorization of the matrix $\tilde{C}^{[0]}$, of bandwidth $2s$.

In general, it appears that the nonzero entries of $C_{n,j}^{[s]}$ obey no recognisable numerical relations: for example, the 6×6 leading principal sub-matrix of $C^{[1]}$ for the Hermite weight is

$$\begin{bmatrix} \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{5}{2}} & 0 & 0 & 0 & 0 \\ \sqrt{\frac{1}{3}} & 0 & \sqrt{\frac{19}{6}} & 0 & 0 & 0 \\ 0 & \sqrt{\frac{3}{5}} & 0 & \sqrt{\frac{39}{10}} & 0 & 0 \\ 0 & 0 & \sqrt{\frac{18}{19}} & 0 & \sqrt{\frac{173}{38}} & 0 \\ 0 & 0 & 0 & \sqrt{\frac{819}{407}} & 0 & \sqrt{\frac{407}{78}} \end{bmatrix}.$$

It is difficult to discern a pattern: numerical experiments for large values of n indicate that both $C_{n,n}^{[1]}$ and $C_{n+2,n}^{[1]}$ grow like $\mathcal{O}(\sqrt{n})$, in line with the proof of the Freud conjecture (Lubinsky, Mhaskar & Saff 1988).

All this does not rule out computing the $C_{n,j}^{[s]}$s numerically. Modifying a weight by a quadratic factor and computing the connection coefficients is discussed in (Gautschi 2004) and (Golub & Meurant 2009).

An alternative approach toward the polynomials $p_n^{[s]}$ uses the *Christoffel theorem* (Ismail 2005, p. 37). Given a measure $\mathrm{d}\mu$ and the corresponding set of *monic* orthogonal polynomials $\{p_n\}_{n\in\mathbb{Z}_+}$, as well as a polynomial $\Xi(\xi) = \prod_{\ell=1}^{r} (\xi - \zeta_\ell)$, the theorem allows for an explicit construction of polynomials orthogonal with respect to

$\Xi(\xi)\,\mathrm{d}\mu(\xi)$. Specialised to the problem at hand, $r = 2s$ and

$$\Xi(x) = \sum_{j=0}^{s} \xi^{2j} = \frac{1-\xi^{2(s+1)}}{1-\xi^2} = \prod_{\substack{\ell=-s\\ \ell\neq 0}}^{s} (\xi - \xi_\ell)$$

where $\xi_\ell = \mathrm{e}^{\mathrm{i}\pi\ell/(s+1)}$, whereby Uvarov's construction yields

$$p_n^{[s]}(\xi) = \frac{1}{h_{n,s}\Xi(\xi)} \det \begin{bmatrix} p_n(\xi_1) & p_{n+1}(\xi_1) & \cdots & p_{n+2s}(\xi_1) \\ p_n(\xi_2) & p_{n+1}(\xi_2) & \cdots & p_{n+2s}(\xi_2) \\ \vdots & \vdots & & \vdots \\ p_n(\xi_s) & p_{n+1}(\xi_s) & \cdots & p_{n+2s}(\xi_s) \\ p_n(\xi) & p_{n+1}(\xi) & \cdots & p_{n+2s}(\xi) \end{bmatrix}, \tag{3.8}$$

where

$$h_{n,s} = \det \begin{bmatrix} p_n(\xi_1) & p_{n+1}(\xi_1) & \cdots & p_{n+2s-1}(\xi_1) \\ p_n(\xi_2) & p_{n+1}(\xi_2) & \cdots & p_{n+2s-1}(\xi_2) \\ \vdots & \vdots & & \vdots \\ p_n(\xi_s) & p_{n+1}(\xi_s) & \cdots & p_{n+2s-1}(\xi_s) \end{bmatrix}.$$

While the polynomials $p_n^{[s]}$ in (3.8) are monic, they can be easily orthonormalised to fit into our setting.

Polynomials of the second cascade display an interesting feature. We recall that an orthogonal polynomial system is *semiclassical* (Hendriksen & van Rossum 1985) if their weight function w obeys the linear differential equation

$$Aw' + Bw = 0, \qquad A, B \text{ polynomials}, \quad A(\xi) > 0 \text{ for } \xi \in \operatorname{supp} w. \tag{3.9}$$

The following lemma is valid *inter alia* for all the examples in the current paper.

Lemma 8 *If* $\mathrm{d}\mu(\xi) = w(\xi)\,\mathrm{d}\xi$ *and* w *obeys (3.9) then all the systems* $\{p_n^{[s]}\}_{n\in\mathbb{Z}_+}$ *for* $s \in \mathbb{Z}_+$ *are semiclassical.*

Proof We include a short proof, but note this result is a special case of Theorem 5.1 of (García-Ardila, Marcellán & Marriaga 2018).

Let $s \in \mathbb{N}$. Set $\Xi_s(\xi) = \prod_{j=0}^{s} \xi^{2j} > 0$, $\xi \in \operatorname{supp} w$, and $w_s = \Xi_s w$. It is trivial to confirm by direct differentiation that

$$A\Xi_s w_s' + (B\Xi_s - A\Xi_s')w_s = 0$$

and $A\Xi_s > 0$, hence w_s is consistent with (3.9) and $\{p_n^{[s]}\}_{n\in\mathbb{Z}_+}$ is semiclassical. □

In other words, semiclassicality is preserved throughout a cascade of the second kind.

4 Hermite-type systems

4.1 The Hermite–Sobolev cascade of the first kind

A natural starting point is the Hermite weight $w(\xi) = \mathrm{e}^{-\xi^2}$, $\xi \in \mathbb{R}$, and $s = 1$. The mollifier, by the definitions in Section 3, is $g(\xi) = \mathrm{e}^{-\xi^2/2}/(1+\xi^2)^{1/2}$, so

$$\varphi_n(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\mathrm{H}}_n(\xi) \sqrt{\frac{\mathrm{e}^{-\xi^2}}{1+\xi^2}} \mathrm{e}^{\mathrm{i}x\xi}\, \mathrm{d}\xi, \qquad n \in \mathbb{Z}_+, \tag{4.1}$$

where

$$\tilde{\mathrm{H}}_n(\xi) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \mathrm{H}_n(\xi), \qquad n \in \mathbb{Z}_+,$$

are the orthonormalised Hermite polynomials. Unfortunately, the integrals (4.1) are not known in an explicit form, not even φ_0.

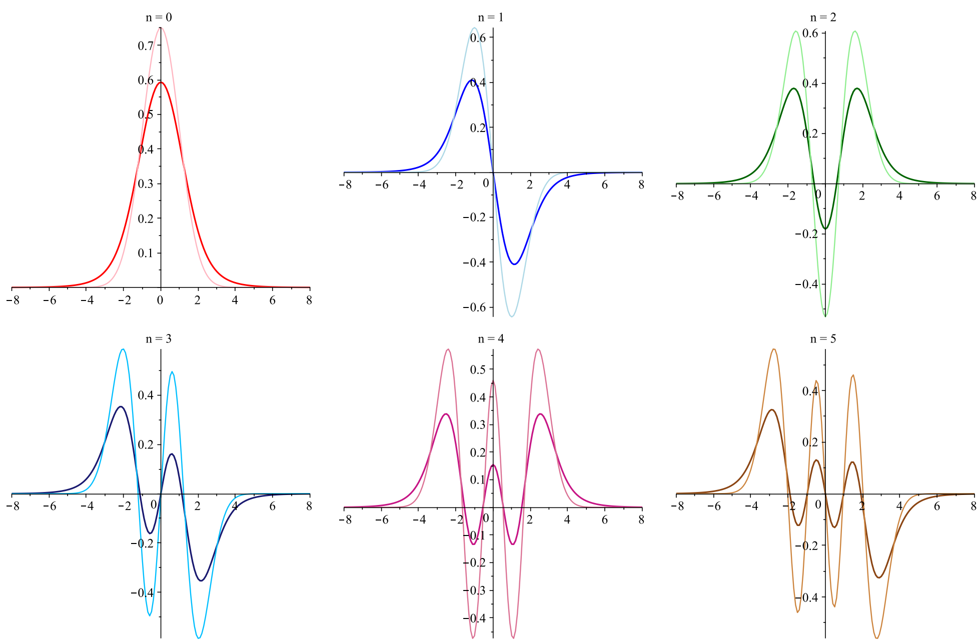

Figure 4.1: The first six functions $\varphi_n^{\langle 1 \rangle}$ defined by (4.1), with corresponding Hermite functions $\varphi_n^{\langle 0 \rangle}(x) = (-1)^n \mathrm{e}^{-x^2/2} \tilde{\mathrm{H}}_n(x)$ in darker shade.

In Fig. 4.1 we display the functions φ_n, $n = 0, \ldots, 5$, computed by brute-force numerical quadrature. In the background, in fainter colour, we display the familiar Hermite functions which follow from (1.1) and are orthonormal in $\mathrm{L}_2(\mathbb{R})$ (while, by Theorem 4, the φ_ns are orthonormal in $\mathbf{H}_2^1(\mathbb{R})$).

4.2 The Hermite–Sobolev cascade of the second kind

While the polynomials $p_n^{[s]}$ from Subsection 3.1 are unknown for $s \in \mathbb{N}$, it is possible to generate them, as explained in Section 3 or directly from the moments: in the simplest nontrivial case, $s = 1$, the moments are

$$\mu_n = \int_{-\infty}^{\infty} \xi^n (1+\xi^2) \mathrm{e}^{-\xi^2}\, \mathrm{d}\xi = \begin{cases} \dfrac{\sqrt{\pi} n!(n+3)}{2^{n+1}\left(\frac{n}{2}\right)!}, & n \text{ even}, \\ 0, & n \text{ odd}, \end{cases}$$

and the first few $p_n^{[1]}$s are

$$\begin{aligned} p_0^{[1]}(\xi) &\equiv \frac{\sqrt{6}}{3\pi^{1/4}}, \\ p_1^{[1]}(\xi) &= \frac{2\sqrt{5}}{5\pi^{1/4}}\xi, \\ p_2^{[1]}(\xi) &= \frac{2\sqrt{57}}{19\pi^{1/4}}\left(\xi^2 - \frac{5}{6}\right), \\ p_3^{[1]}(\xi) &= \frac{2\sqrt{130}}{39\pi^{1/4}}\left(\xi^3 - \frac{21}{10}\xi\right), \\ p_4^{[1]}(\xi) &= \frac{2\sqrt{9861}}{519\pi^{1/4}}\left(\xi^4 - \frac{75}{19}\xi^2 + \frac{117}{76}\right), \\ p_5^{[1]}(\xi) &= \frac{2\sqrt{52910}}{2035\pi^{1/4}}\left(\xi^5 - \frac{245}{39}\xi^3 + \frac{335}{52}\xi\right) \end{aligned}$$

and so on. Likewise, it is possible to compute recurrence coefficients,

$$b_0 = \sqrt{\frac{5}{6}},\ b_1 = \sqrt{\frac{19}{15}},\ b_2 = \sqrt{\frac{315}{190}},\ b_3 = \sqrt{\frac{1730}{741}},\ b_4 = \sqrt{\frac{38665}{13494}},\ b_5 = \sqrt{\frac{236925}{70411}}$$

etc. but difficult to discern any pattern except for the obvious, $b_n = \mathcal{O}\big(n^{1/2}\big)$, $n \gg 1$, a consequence of the proof of the Freud conjecture in (Lubinsky et al. 1988). Likewise, we can compute $p_n^{[s]}$ for $s \geq 2$: Fig. 4.2 displays $p_n^{[s]}$ for $n = 2, 3, 4, 5$ and $s = 0, 1, 2, 3, 4$.

Computing the $\varphi_n^{[1]}$s in line with (1.5) is straightforward:

$$\begin{aligned} \varphi_0^{[1]}(x) &= \sqrt{\frac{2}{3}}\pi^{-1/4}\mathrm{e}^{-x^2/2}, \\ \varphi_1^{[1]}(x) &= -\sqrt{\frac{4}{5}}\pi^{-1/4}x\mathrm{e}^{-x^2/2}, \\ \varphi_2^{[1]}(x) &= \frac{1}{\sqrt{57}}\pi^{-1/4}(6x^2-1)\mathrm{e}^{-x^2/2}, \\ \varphi_3^{[1]}(x) &= -\sqrt{\frac{2}{585}}\pi^{-1/4}(10x^3-9x)\mathrm{e}^{-x^2/2}, \\ \varphi_4^{[1]}(x) &= \frac{1}{\sqrt{39444}}\pi^{-1/4}(76x^4-156x^2+45)\mathrm{e}^{-x^2/2}, \end{aligned}$$

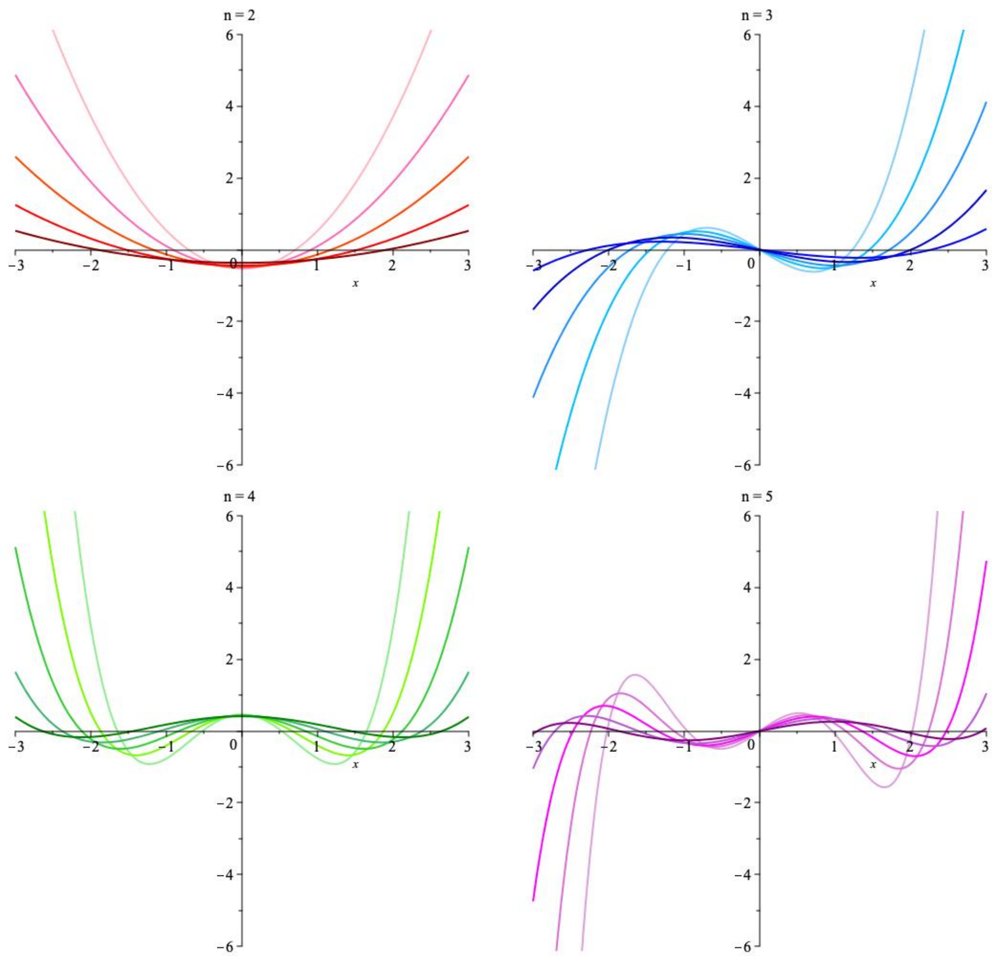

Figure 4.2: The polynomials $p_n^{[s]}$ for $n = 2, 3, 4, 5$ and $s = 0, 1, 2, 4$ (darker hue corresponds to larger s).

$$\varphi_5^{[1]}(x) = -\frac{1}{\sqrt{476190}}\pi^{-1/4}(156x^5 - 580x^3 + 405x)\mathrm{e}^{-x^2/2}$$

and so on.

Fig. 4.3 displays the above functions $\varphi_n^{[1]}$ and, in fainter colour, the functions $\varphi_n^{\langle 0\rangle}$ based on the same weight $w(\xi) = (1+\xi^2)\mathrm{e}^{-\xi^2}$ and defined by (1.1).

Lemma 9 *For every $n \in \mathbb{Z}_+$ we have $\varphi_n^{[1]}(x) = \lambda_n(x)\mathrm{e}^{-x^2/2}$, where λ_n is an nth-degree polynomial.*

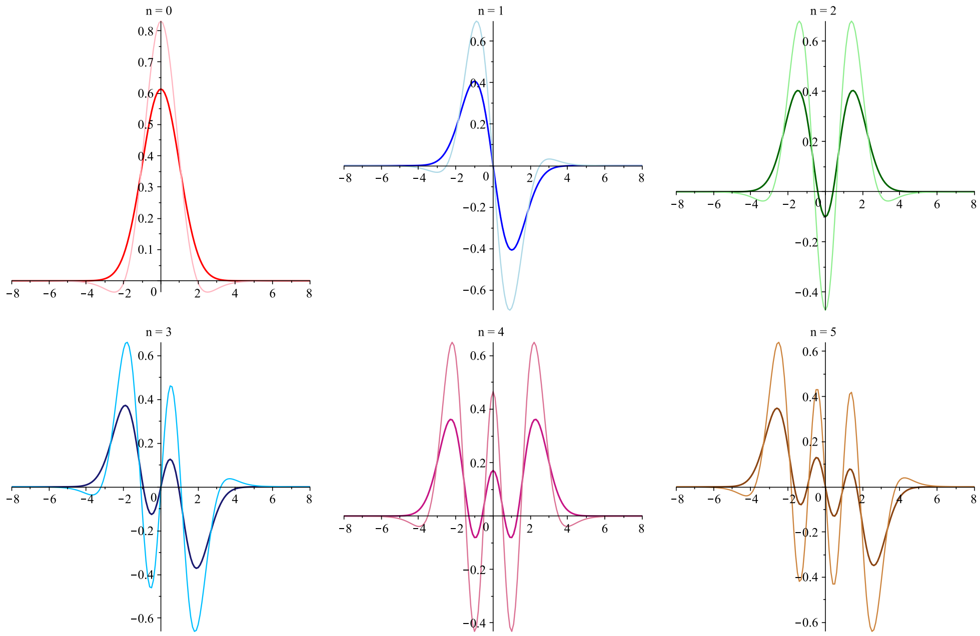

Figure 4.3: The first six functions $\varphi_n^{[1]}$ with corresponding functions $\varphi_n^{[0]}$, which are orthogonal in $\mathrm{L}_2(\mathbb{R})$, in darker shade.

Proof It is enough to prove that

$$\sigma_n(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \xi^n \mathrm{e}^{-\xi^2/2+\mathrm{i}x\xi} \,\mathrm{d}\xi, \qquad n \in \mathbb{Z}_+,$$

is of the asserted form, i.e. an nth degree polynomial times $\mathrm{e}^{-x^2/2}$. This follows readily by induction on n from $\sigma_0(x) = \mathrm{e}^{-x^2/2}$ and $\sigma_n' = \sigma_{n+1}$ because, letting $\sigma_n(x) = \alpha_n(x)\mathrm{e}^{-x^2/2}$, we obtain $\alpha_{n+1}(x) = \alpha_n'(x) - x\alpha_n(x)$. □

Alternatively, substituting into (2.1), it is easy to see that

$$\lambda_n'(x) = -b_{n-1}\lambda_{n-1}(x) + x\lambda_n(x) + b_n\lambda_{n+1}(x), \qquad n \in \mathbb{Z}_+.$$

The proof that λ_n is an nth degree polynomial follows at once by induction on this differential recurrence, since $b_n > 0$, $n \in \mathbb{N}$.

The bad news is that the λ_ns are not known and, as is trivial to verify, they do not obey a three-term recurrence relation (hence, by the Favard theorem, cannot be orthogonal with respect to any Borel measure). However, intriguingly, it follows easily from $\mathbf{H}_2^1$ orthogonality of the $\varphi_n^{[1]}$s that the λ_n are orthogonal with regard to the unconventional inner product

$$\langle f, g \rangle = \int_{-\infty}^{\infty} \{(1+x^2)f(x)g(x) - x[f'(x)g(x) + f(x)g'(x)] + f'(x)g'(x)]\,\mathrm{d}x.$$

It has been proved in (Iserles & Webb 2019) that there exists a unique L_2-orthonormal system on the real line which obeys (1.2) and where each function is a polynomial multiple of the same L_2 function, specifically Hermite functions (or $\varphi_n^{[0]} = \varphi_n^{\langle 0\rangle}$ in present notation). The functions $\{\varphi_n^{[1]}\}_{n\in\mathbb{Z}_+}$, though, are $\mathbf{H}_2^1$-orthonormal, they obey (1.2) and $\varphi_n^{[1]}(x) = \mathrm{e}^{-x^2/2}\lambda_n(x)$.

Lemma 10 *The only $\mathbf{H}_{2,v}(\mathbb{R})$-orthonormal systems (see equation (1.7)) with a tridiagonal differentiation matrix which are of the form $\varphi_n(x) = G(x)\lambda_n(x)$, $n \in \mathbb{Z}_+$, for some function $G \in L_2(\mathbb{R})$, $G > 0$ (and $G(0) = 1$ without loss of generality), where each λ_n is a polynomial of degree n, correspond to*

$$G(x) = \exp\left(-\gamma x^2 + \delta x\right) \tag{4.2}$$

for some constants $\gamma > 0$ and $\delta \in \mathbb{R}$. The corresponding weight of orthonormality for P in Theorem 1 is

$$w(\xi) \propto v(\xi)\mathrm{e}^{-\xi^2/(2\gamma)}. \tag{4.3}$$

Proof We substitute $\varphi_n(x) = G(x)\lambda_n(x)$ into (2.1), bearing in mind that $G > 0$, to obtain,

$$\lambda_n'(x) = -b_{n-1}\lambda_{n-1}(x) + \left[\mathrm{i}c_n - \frac{G'(x)}{G(x)}\right]\lambda_n(x) + b_n\lambda_{n+1}(x), \qquad n \in \mathbb{Z}_+.$$

Since $\deg \lambda_m = m$ by assumption, we deduce, comparing degrees, that G'/G is a linear polynomial, and hence that $G(x)$ is the exponential of a quadratic polynomial. We can set the constant term in this quadratic to zero since $G(0) = 1$ without loss of generality, so we obtain equation (4.2).

Inverting the representation in Theorem 1, we have

$$p_n(\xi)g(\xi) = \frac{(-\mathrm{i})^n}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\varphi_n(x)\mathrm{e}^{-\mathrm{i}x\xi}\,\mathrm{d}x = \frac{(-\mathrm{i})^n}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\lambda_n(x)\mathrm{e}^{-\gamma x^2\xi+\delta x-\mathrm{i}x\xi}\,\mathrm{d}x.$$

The case $n = 0$ tells us that

$$g(\xi) \propto \exp(-(\xi - \mathrm{i}\delta)^2/(4\gamma)). \tag{4.4}$$

Theorem 4 tells us that for $\mathbf{H}_{2,v}(\mathbb{R})$ orthonormality we require

$$w(\xi) = v(\xi)|g(\xi)|^2, \tag{4.5}$$

which completes the proof of necessity of the forms of G and w.

Now we prove sufficiency. Let $w(\xi) = C^2v(\xi)\mathrm{e}^{-\xi^2/2\gamma}$ where C ensures w has unit integral, $g(\xi) = C\mathrm{e}^{-(\xi-\mathrm{i}\delta)^2/(4\gamma)}$, and define Φ as in Theorem 1. By Theorem 4, Φ is an $\mathbf{H}_{2,v}(\mathbb{R})$-orthonormal system, so all that remains to prove is that $\varphi_n(x) = G(x)\lambda_n(x)$ where λ_n is a polynomial of degree n. It is sufficient to show that $\rho_n(x) = \int_{-\infty}^{\infty}\xi^n g(\xi)\mathrm{e}^{\mathrm{i}x\xi}\,\mathrm{d}\xi$ is $G(x)$ times a polynomial of degree n, which can be readily shown by induction starting from $\rho_0(x) \propto G(x)$ and leveraging $\rho_{n+1}(x) = -\mathrm{i}\rho_n'(x)$. □

4.3 An $\mathbf{H}_2^\infty(\mathbb{R})$ system based on the Hermite weight

Let $\sigma\in(0,1)$, $w(\xi)=\mathrm{e}^{-\xi^2}$ (i.e. the standard Hermite weight) and $v(\xi)=\mathrm{e}^{\sigma\xi^2}$, $\xi\in\mathbb{R}$. Therefore, by Theorem 3, the functions φ_n, as defined by (2.3), are orthogonal with respect to the infinite Sobolev inner product

$$\langle f,g\rangle_v=\sum_{\ell=0}^{\infty}\frac{\sigma^\ell}{\ell!}\int_{-\infty}^{\infty}f^{(\ell)}(x)g^{(\ell)}(x)\,\mathrm{d}x. \tag{4.6}$$

In this case p_ns are scaled Hermite polynomials and φ_ns can be computed explicitly.

Theorem 11 *The Hermite weight $w(\xi)=\mathrm{e}^{-\xi^2}$, $x\in\mathbb{R}$, generates the $\mathbf{H}_2^\infty(\mathbb{R})$ system*

$$\varphi_n^{[\infty]}(x)=\frac{1}{\sqrt{1+\sigma}}\left(\frac{1-\sigma}{1+\sigma}\right)^{n/2}\varphi_n^{[0]}\left(\frac{x}{\sqrt{1-\sigma^2}}\right)\exp\left(\frac{\sigma x^2}{2(1-\sigma^2)}\right),\qquad n\in\mathbb{Z}_+, \tag{4.7}$$

where $\varphi_n^{[0]}$ is the standard nth Hermite function.

Proof Let

$$\tilde{\varphi}_n(x)=\frac{\mathrm{i}^n}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{H}_n(\xi)\mathrm{e}^{-\frac{1}{2}(1+\sigma)\xi^2+\mathrm{i}x\xi}\,\mathrm{d}\xi,\qquad n\in\mathbb{Z}_+,$$

whereby, orthonormalising Hermite polynomials, (2.3) yields $\varphi_n(x)=\tilde{\varphi}_n(x)/\sqrt{2^n n!\sqrt{\pi}}$. Using the standard generating function for Hermite polynomials,

$$\begin{aligned}\sum_{n=0}^{\infty}\frac{\tilde{\varphi}_n(x)}{n!}t^n&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\sum_{n=0}^{\infty}\frac{\mathrm{H}_n(\xi)}{n!}(\mathrm{i}t)^n\right]\exp\left(-\frac{1+\sigma}{2}\xi^2+\mathrm{i}x\xi\right)\mathrm{d}\xi\\
&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\left(2\mathrm{i}\xi t+t^2-\frac{1+\sigma}{2}\xi^2+\mathrm{i}x\xi\right)\mathrm{d}\xi\\
&=\frac{1}{\sqrt{1+\sigma}}\exp\left(-\frac{x^2}{2(1+\sigma)}\right)\exp\left(-\frac{2xt}{1+\sigma}-\frac{1-\sigma}{1+\sigma}t^2\right)\\
&=\frac{1}{\sqrt{1+\sigma}}\exp\left(-\frac{x^2}{2(1+\sigma)}\right)\exp\left(-\frac{2x}{\sqrt{1-\sigma^2}}\left(\sqrt{\frac{1-\sigma}{1+\sigma}}t\right)-\left(\sqrt{\frac{1-\sigma}{1+\sigma}}t\right)^2\right)\end{aligned}$$

and, using the same generating function in the opposite direction,

$$\sum_{n=0}^{\infty}\frac{\tilde{\varphi}_n(x)}{n!}t^n=\frac{1}{\sqrt{1+\sigma}}\exp\left(-\frac{x^2}{2(1+\sigma)}\right)\sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{H}_n\left(-\frac{x}{\sqrt{1-\sigma^2}}\right)\left(\sqrt{\frac{1-\sigma}{1+\sigma}}t\right)^n.$$

Therefore

$$\tilde{\varphi}_n(x)=\frac{(-1)^n}{\sqrt{1+\sigma}}\left(\frac{1-\sigma}{1+\sigma}\right)^{n/2}\mathrm{H}_n\left(\frac{x}{\sqrt{1-\sigma^2}}\right)\exp\left(-\frac{x^2}{2(1+\sigma)}\right).$$

Normalising,

$$\varphi_n^{[\infty]}(x) = \frac{(-1)^n}{\sqrt{(1+\sigma)2^n n!\sqrt{\pi}}} \left(\frac{1-\sigma}{1+\sigma}\right)^{n/2} \mathrm{H}_n\left(\frac{x}{\sqrt{1-\sigma^2}}\right) \exp\left(-\frac{x^2}{2(1+\sigma)}\right),$$
$$= \frac{1}{\sqrt{1+\sigma}} \left(\frac{1-\sigma}{1+\sigma}\right)^{n/2} \varphi_n^{[0]}\left(\frac{x}{\sqrt{1-\sigma^2}}\right) \exp\left(\frac{\sigma x^2}{2(1-\sigma^2)}\right), \qquad n \in \mathbb{Z}_+,$$

and (4.7) is true. □

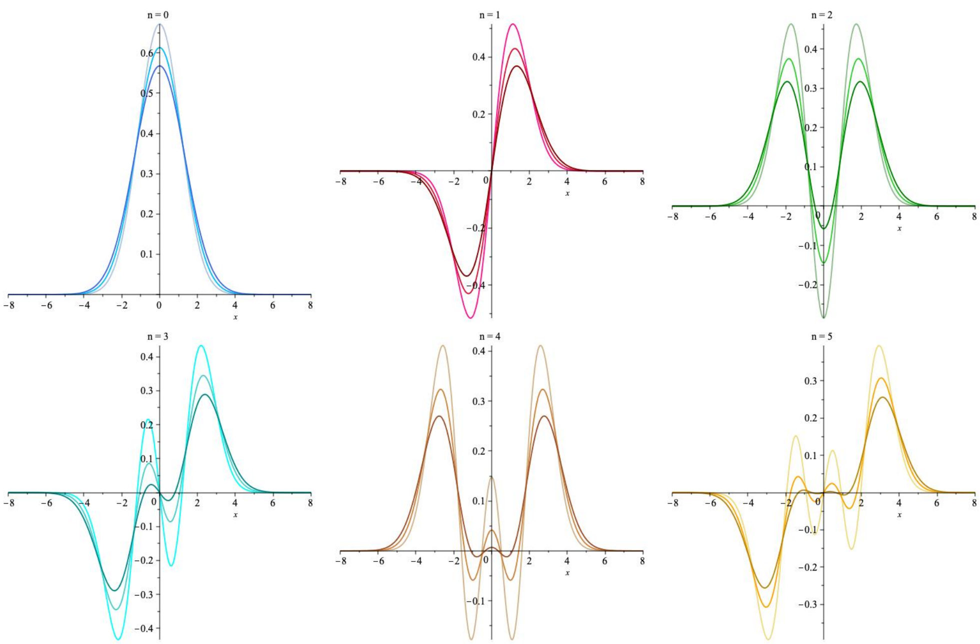

Figure 4.4: The first six $\mathbf{H}_2^\infty$ Hermite-type functions $\varphi_n^{[\infty]}$ for $\sigma = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ in progressively darker hues.

Fig. 4.4 displays the functions $\varphi_n^{[\infty]}$, $n = 0, \ldots, 5$, for three different values of $\sigma \in (0,1)$. The zeros of φ_n are scaled zeros of a Hermite polynomial and, the scaling being monotone, the zeros are 'squeezed' in a uniform manner for increasing σ, as evident in the figure.

5 Bilateral Laguerre-type weights

Deferring the standard Laguerre weight (which is not symmetric) to Section 7, we let $w(\xi) = (1+\xi^2)\mathrm{e}^{-|\xi|}$, $\xi \in \mathbb{R}$. Note that the underlying orthogonal polynomials are unknown explicitly, yet can be computed. The $\varphi_n^{[1]}$s are

$$\varphi_0^{[1]}(x) = \frac{2}{\sqrt{3}\sqrt{\pi}}\frac{1}{1+4x^2},$$

$$\varphi_1^{[1]}(x) = \frac{16}{\sqrt{26}\sqrt{\pi}}\frac{x}{(1+4x^2)^2},$$

$$\varphi_2^{[1]}(x) = \frac{2}{\sqrt{1167}\sqrt{\pi}}\frac{1+248x^2+208x^4}{(1+4x^2)^3},$$

$$\varphi_3^{[1]}(x) = \frac{16}{\sqrt{23179}\sqrt{\pi}}\frac{-21x+456x^3+496x^5}{(1+4x^2)^4},$$

$$\varphi_4^{[1]}(x) = \frac{2}{\sqrt{309347971}\sqrt{\pi}}\frac{2925-128784x^2+1703264x^4+3029760x^6+1369344x^8}{(1+4x^2)^5},$$

$$\varphi_5^{[1]}(x) = \frac{16}{\sqrt{22678864934}\sqrt{\pi}}\frac{25749x-1017424x^3+5715040x^5+13510400x^7+7744768x^9}{(1+4x^2)^6}.$$

The general formula is a polynomial of degree $2n-[1-(-1)^n]/2$ in x (of the same parity as n), divided by $(1+4x^2)^{n+1}$. This can be easily verified because by (2.3) and $g(\xi)=\mathrm{e}^{-|\xi|/2}$ each $\varphi_n^{[1]}$ is a linear combination of $\lambda_n, \lambda_{n-2}, \ldots$, where

$$\lambda_n(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \xi^n \mathrm{e}^{-|\xi|^2+\mathrm{i}x\xi}\,\mathrm{d}\xi, \qquad n\in\mathbb{Z}_+$$

and $\lambda_n'(x)=\lambda_{n+1}(x)$ implies that

$$\lambda_n(x) = \lambda_0^{(n)}(x) = \frac{2\sqrt{2}}{\sqrt{\pi}}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\frac{1}{1+4x^2}, \qquad n\in\mathbb{Z}_+.$$

6 Bessel-like functions

6.1 Transformation of Chebyshev polynomials

We rewrite (1.6) in the form (2.3),

$$\varphi_n(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}}\int_{-1}^{1}\tilde{\mathrm{T}}_n(\xi)\mathrm{e}^{\mathrm{i}x\xi}\frac{\mathrm{d}\xi}{\sqrt{1-\xi^2}} = (-1)^n \mathrm{J}_n(x),$$

where $\tilde{\mathrm{T}}_n = \sqrt{2/\pi}\mathrm{T}_n$ (except that $\tilde{\mathrm{T}}_0 \equiv \mathrm{T}_0/\sqrt{\pi}$) are orthonormal Chebyshev polynomials of the first kind. It is easy to verify directly that the φ_ns cannot be bounded in *any* Sobolev norm because the Weber–Schafheitlin formula (Olver, Lozier, Boisvert & Clark 2010, 10.22.57) implies that for $\mathrm{Re}\,\lambda>0$

$$\int_{-\infty}^{\infty}\frac{\varphi_n^2(x)\,\mathrm{d}x}{x^\lambda} = \int_{-\infty}^{\infty}\frac{\mathrm{J}_n^2(x)\,\mathrm{d}x}{x^\lambda} = \frac{\Gamma(n+\frac12)\Gamma(\lambda)}{2^{\lambda-1}\Gamma^2(\frac12\lambda+\frac12)\Gamma(\frac12\lambda+n+\frac12)} \xrightarrow{\lambda\to0} \infty.$$

If instead of a Chebyshev measure we use the Legendre measure, $w(\xi)=\chi_{(-1,1)}(\xi)$, the state of affairs is different: $g(\xi)=\chi_{(-1,1)}$ results in

$$\varphi_n(x) = (-1)^n\sqrt{\frac{n+\frac12}{x}}\mathrm{J}_{n+\frac12}(x), \qquad x\in\mathbb{R}, \tag{6.1}$$

and the φ_ns are integrable on $\mathbb{R}$.

6.2 The Legendre weight

The most obvious example of an $\mathbf{H}_2^1(\mathbb{R})$ system is based on the Legendre weight $w(\xi) = \chi_{(-1,1)}(\xi)$, in which the orthonormal polynomials are $p_n = \sqrt{n+\frac{1}{2}}\mathrm{P}_n$. Thus,

$$\varphi_n^{\langle 1\rangle}(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}}\sqrt{n+\frac{1}{2}}\int_{-1}^{1}\frac{\mathrm{P}_n(\xi)}{\sqrt{1+\xi^2}}\mathrm{e}^{\mathrm{i}x\xi}\,\mathrm{d}\xi, \qquad n\in\mathbb{Z}_+.$$

While $\{\varphi_n^{\langle 1\rangle}\}_{n\in\mathbb{Z}_+}$ is orthonormal in $\mathbf{H}_2^1(\mathbb{R})$, it is not a complete basis because all Fourier spectra are restricted to $[-1,1]$, yet it might be of an independent interest. Perhaps a more vexing issue is that above integrals are not available in an explicit form. This is not an insurmountable problem in the computation of the $\varphi_n^{\langle 1\rangle}$s which we can compute for individual values of x using a Fast Fourier Transform (Townsend, Webb & Olver 2018, Olver, Slevinsky & Townsend 2020), although it presents an obvious obstacle to their analysis.

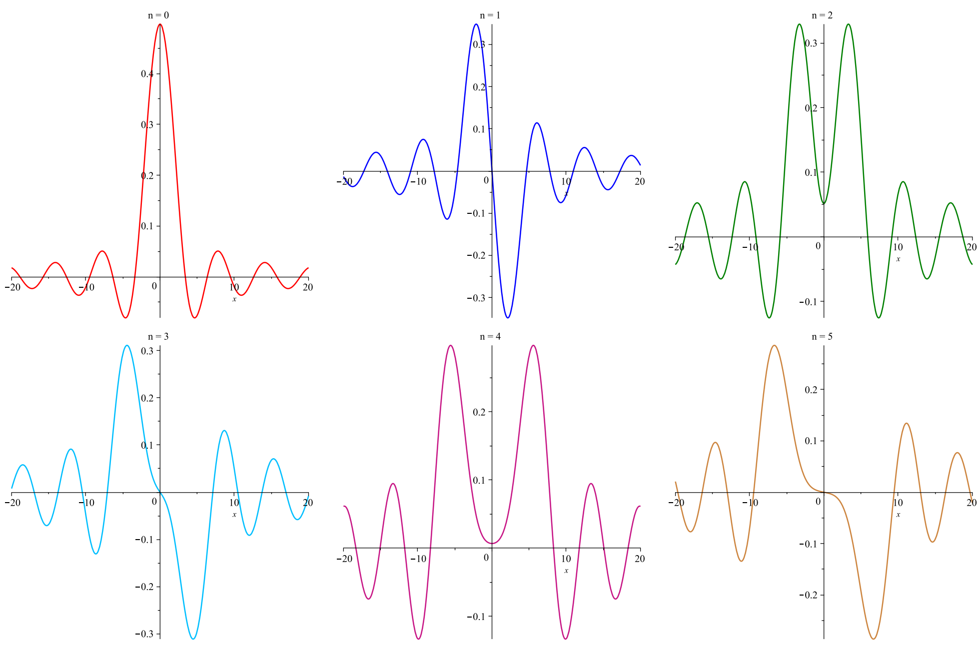

Figure 6.1: The first six functions $\varphi_n^{\langle 1\rangle}$ for the Legendre weight.

In Fig. 6.1 we have computed $\varphi_0^{\langle 1\rangle},\ldots,\varphi_5^{\langle 1\rangle}$ numerically. Like other transformed functions (1.1) or (2.3), the $\varphi_n^{\langle 1\rangle}$s seem to be endowed with a wealth of structural features and regularities which have been discussed briefly (for (1.1)) in (Iserles & Webb 2021*a*) but overall are a subject for future research.

6.3 Sobolev–Legendre cascades

We revisit the essence of Subsections 3.1.1–2, except that the range of integration is now $[-1,1]$. Firstly, we set $w=\chi_{(-1,1)}$, let p_n be the (orthonormalised) Legendre polynomials and, for every $s\in\mathbb{Z}_+$ set

$$\varphi_n^{\langle s\rangle}(x)=\frac{\mathrm{i}^n}{\sqrt{2\pi}}\int_{-1}^{1}p_n(\xi)\left(\sum_{\ell=0}^{s}\xi^{2\ell}\right)^{-1/2}\mathrm{e}^{\mathrm{i}x\xi}\,\mathrm{d}\xi,\qquad n\in\mathbb{Z}_+. \tag{6.2}$$

Secondly, we might define $w_s(\xi)=\chi_{(-1,1)}(\xi)\sum_{\ell=0}^{s}\xi^{2\ell}$, $s\in\mathbb{Z}_+$, and set

$$\varphi_n^{[s]}(x)=\frac{\mathrm{i}^n}{\sqrt{2\pi}}\int_{-1}^{1}p_n^{[s]}(\xi)\mathrm{e}^{\mathrm{i}x\xi}\,\mathrm{d}\xi,\qquad n\in\mathbb{Z}_+, \tag{6.3}$$

where $\{p_n^{[s]}\}_{n\in\mathbb{Z}_+}$ is the orthonormal polynomial system corresponding to the weight w_s. It follows at once from Theorem 4 that

$$\sum_{\ell=0}^{s}\int_{-\infty}^{\infty}\frac{\mathrm{d}^\ell\varphi_m^{\langle s\rangle}(x)}{\mathrm{d}x^\ell}\frac{\mathrm{d}^\ell\varphi_n^{\langle s\rangle}(x)}{\mathrm{d}x^\ell}\,\mathrm{d}x=\sum_{\ell=0}^{s}\int_{-\infty}^{\infty}\frac{\mathrm{d}^\ell\varphi_m^{[s]}(x)}{\mathrm{d}x^\ell}\frac{\mathrm{d}^\ell\varphi_n^{[s]}(x)}{\mathrm{d}x^\ell}\,\mathrm{d}x=\delta_{m,n}$$

for all $m,n\in\mathbb{Z}_+$ and both $\{\varphi_n^{\langle s\rangle}\}_{n\in\mathbb{Z}_+}$ and $\{\varphi_n^{[s]}\}_{n\in\mathbb{Z}_+}$ are orthonormal sets in $\mathbf{H}_2^s(\mathbb{R})$. Of course, neither is dense in the Sobolev space because their Fourier spectra are restricted to $[-1,1]$ – they are dense in an obvious generalisation of Paley–Wiener spaces to the realm of Sobolev spaces. The systems (6.2) and (6.3) are the *Sobolev–Legendre cascades* of *the first* and *the second kind,* respectively.

We recall a major practical difference between the two cascades: except for the case $s=0$ (when $\varphi_n^{\langle 0\rangle}=\varphi_n^{[0]}$ has been given in (6.1)), $\varphi_n^{\langle s\rangle}$ is unknown in an explicit form while $\varphi_n^{[s]}$, being an integral in $[-1,1]$ of a polynomial times $\mathrm{e}^{\mathrm{i}x\xi}$, can be computed at great ease and is a linear combination of spherical Bessel functions. Consequently, in the sequel we focus on the Sobolev–Legendre cascade of the second kind.

Fig. 6.2 displays the beginning (that is, $s=0,1,2$) of the cascade of the second kind. The obvious observation is that $\varphi_0^{[s]}$ is a scalar multiple of $\varphi_0^{[0]}$ and the same is true for $\varphi_1^{[s]}$ and $\varphi_1^{[0]}$, respectively. This follows from (6.3) because $p_0^{[s]}$ is a constant, while $p_1^{[s]}$ is a scalar multiple of ξ. Another obvious indication is that, as s grows, $\varphi_n^{[s]}$ converges pointwise to a function $\varphi_n^{[\infty]}$ yet this might be less interesting than it appears. In particular,

Lemma 12 $\varphi_n^{[\infty]}\equiv 0$.

Proof Let

$$u_s=\int_{-1}^{1}\sum_{\ell=0}^{s}\xi^{2\ell}\,\mathrm{d}\xi,\qquad s\in\mathbb{Z}_+.$$

Then $p_0^{[0]}\equiv 1/\sqrt{u_2}$ and, by (6.3),

$$\varphi_0^{[s]}(x)=\sqrt{\frac{2}{\pi u_s}}\frac{\sin x}{x}.$$

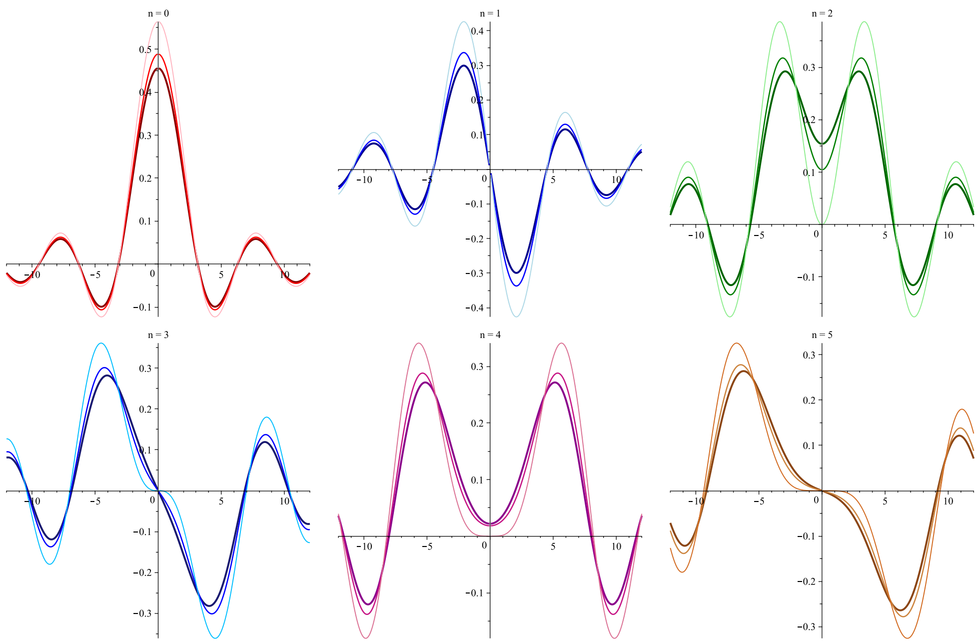

Figure 6.2: The Sobolev–Legendre cascade of the second kind: The first six functions $\varphi_n^{[s]}$ for $s = 0, 1, 2$: increasing s corresponds to increasing line thickness and darker hue.

But

$$u_s = \sum_{\ell=0}^{s} \frac{1}{\ell + \frac{1}{2}} \stackrel{\ell\to\infty}{\longrightarrow} \infty$$

and the lemma follows. □

Alternatively, $\lim_{s\to\infty} w^{[s]}(\xi) = (1-\xi^2)^{-1}\chi_{(-1,1)} \notin \mathrm{L}_2(\mathbb{R})$. An obvious remedy, which we do not pursue in this paper, is to consider the weight $w_s(\xi) = \sum_{\ell=0}^{s} \sigma^\ell \xi^{2\ell}$ for some $\sigma \in (0, 1)$.

6.4 The Sobolev-ultraspherical cascade of the second kind

We construct a cascade of the second kind based on the ultraspherical weight $w^{[0]}(\xi) = (1-\xi^2)\chi_{(-1,1)}(\xi)$. Therefore

$$w^{[s]}(\xi) = w^{[0]}(\xi) \sum_{\ell=0}^{s} \xi^{2\ell} = (1-\xi^{2s+2})\chi_{(-1,1)}, \qquad s \in \mathbb{Z}_+$$

and, as $s \to \infty$, $w^{[s]}$ converges weakly to the Legendre weight.

In Fig. 6.3 we display the functions $\varphi_n^{[0]}, \ldots, \varphi_n^{[3]}$ for $n = 0, 1, \ldots, 5$. While the convergence to a limit in each figure is quite persuasive, we must beware of 'proof by

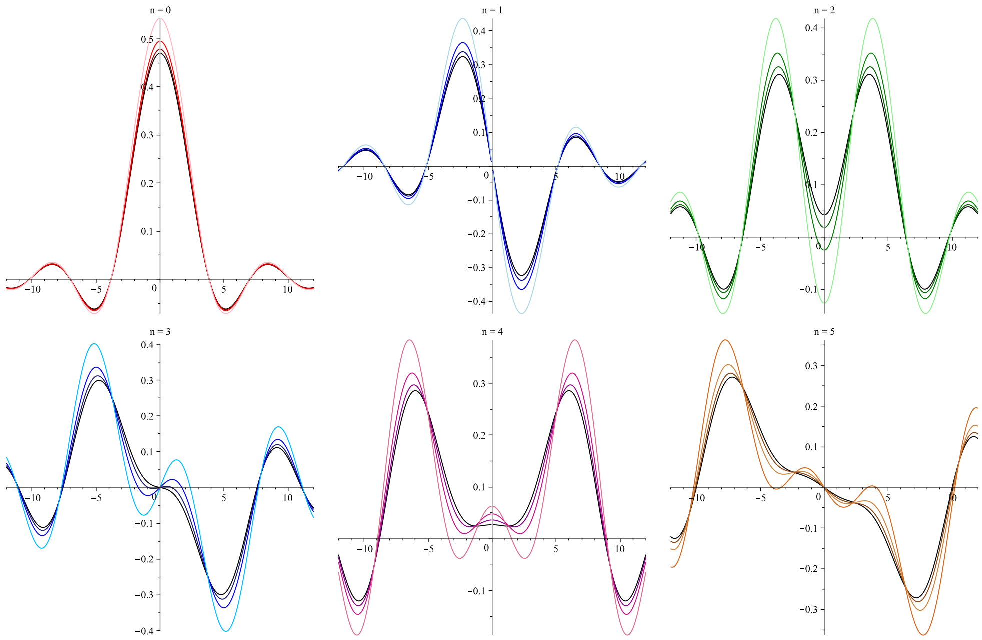

Figure 6.3: The Sobolev–ultrasperical cascade: The first six functions $\varphi_n^{[s]}$ for $s = 0, 1, 2, 3$: increasing s corresponds to darker hue.

picture': convergence is equally pictorially persuasive in Fig. 6.2 where, as we have already seen, it need not take place.

7 Non-symmetric measures

The most obvious non-symmetric weight function is the Laguerre weight $w(\xi) = \mathrm{e}^{-\xi}\chi_{[0,\infty)}(\xi)$. In that case the φ_ns are the *Malmquist–Takenaka functions,* which have a particularly neat form,

$$\varphi_n(x) = \sqrt{\frac{2}{\pi}}\mathrm{i}^n \frac{(1+2\mathrm{i}x)^n}{(1-2\mathrm{i}x)^{n+1}}, \qquad n \in \mathbb{Z}_+, \tag{7.1}$$

(Iserles & Webb 2020), and they are dense in $\mathcal{PW}_{[0,\infty)}(\mathbb{R})$. It is possible to extend them to a system dense in all of $\mathrm{L}_2(\mathbb{R})$ by melding them with another system, generated by the mirror image of the Laguerre weight, $\mathrm{e}^{\xi}\chi_{(-\infty,0]}(\xi)$: together we obtain the same system as (7.1), except that now n ranges over all of $\mathbb{Z}$.

It is, of course, perfectly possible for a system with a non-symmetric measure to be dense in $\mathrm{L}_2(\mathbb{R})$, provided that the support of w is all of $\mathbb{R}$: an example is the Hermite-type weight $w(\xi) = (1-\xi)^2\mathrm{e}^{-\xi^2}$.

7.1 Shifted Hermite weight

Letting $\rho \in \mathbb{R}$, we consider the weight $w(\xi) = \mathrm{e}^{-(\xi-\rho)^2}$. The underlying orthonormal polynomials are $p_n(\xi) = \tilde{\mathrm{H}}_n(\xi - \rho)$, where $\tilde{\mathrm{H}}_n$ is the orthonormalised Hermite polynomial, $\tilde{\mathrm{H}}_n = \mathrm{H}_n/\sqrt{2^n n!\sqrt{\pi}}$. Therefore, seeking $\mathbf{H}_2^1(\mathbb{R})$ orthogonality,

$$\varphi_n^{\langle 0\rangle}(x,\rho) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\mathrm{H}}_n(\xi-\rho)\mathrm{e}^{-(\xi-\rho)^2/2+\mathrm{i}x\xi}\,\mathrm{d}\xi = \mathrm{e}^{\mathrm{i}\rho x}\varphi_n^{\langle 0\rangle}(x,0),$$

$$\varphi_n^{\langle 1\rangle}(x,\rho) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\mathrm{H}}_n(\xi-\rho)\frac{\mathrm{e}^{-(\xi-\rho)^2/2+\mathrm{i}x\xi}}{\sqrt{1+\xi^2}}\,\mathrm{d}\xi, \qquad n \in \mathbb{Z}_+.$$

It is easy to verify that

$$\varphi_n^{\langle 0\rangle}(x,\rho) = \mathrm{e}^{\mathrm{i}\rho x}\varphi_0^{\langle 0\rangle}(x,0), \qquad x,\rho \in \mathbb{R}.$$

Thus, $\varphi_n^{\langle 0\rangle} = \varphi_n^{[0]}$ is merely a complex-valued rotation of the standard Hermite function. The situation is more intriguing with regard to $\varphi_n^{\langle 1\rangle}$. Shifting the variable of integration,

$$\varphi_n^{\langle 1\rangle}(x,\rho) = \frac{\mathrm{i}^n \mathrm{e}^{\mathrm{i}\rho x}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\mathrm{H}}_n(\xi)\sqrt{\frac{\mathrm{e}^{-\xi^2}}{1+(\sigma+\xi)^2}}\mathrm{e}^{\mathrm{i}x\xi}\,\mathrm{d}\xi.$$

On the face of it, we recover an expression similar to (2.3), except that $v(\xi) = 1 + (\sigma+\xi)^2$ is not an even function and does not define a Sobolev inner product.

Fig. 7.1 displays the absolute and real values of the complex-valued functions $\varphi_n^{\langle 1\rangle}$.

7.2 The Laguerre weight

7.2.1 Sobolev–Laguerre functions of first kind

Let $w(\xi) = \mathrm{e}^{-\xi}\chi_{[0,\infty)}(\xi)$, a Laguerre weight. Thus, the $\varphi_n^{\langle 0\rangle}$s are Malmquist–Takenaka functions (7.1), which we need to complement with their 'reflections' for $n \in -\mathbb{N}$ to form a system dense in $\mathrm{L}_2(\mathbb{R})$. By similar token, we need to complement $\varphi_n^{\langle 1\rangle}$s, $n \in \mathbb{Z}_+$, with functions generated with $w(\xi) = \mathrm{e}^{\xi}\chi_{(-\infty,0]}(\xi)$ (and indexed by $n \in -\mathbb{N}$) to attain completeness in $\mathbf{H}_2^1(\mathbb{R})$.

It is possible to compute individual $\varphi_n^{\langle 1\rangle}$s explicitly in terms of Bessel functions of the second kind (a.k.a. Weber functions) Y_n (Olver et al. 2010, 10.2.4) and Struve functions $\mathbf{H}_n$ (Olver et al. 2010, 11.2.1). We first let

$$z = \frac{1}{2} - \mathrm{i}x, \qquad g(z) = \mathrm{Y}_0(z) - \mathbf{H}_0(z).$$

The functions φ_n can be represented explicitly as linear combinations of derivatives of the function g.

Lemma 13 *The explicit form of the functions* $\varphi_n^{\langle 1\rangle}$ *is*

$$\varphi_n^{\langle 1\rangle}(x) = -\frac{\sqrt{2\pi}}{4}\mathrm{i}^n \sum_{\ell=0}^{n} \binom{n}{\ell}\frac{1}{\ell!}g^{(\ell)}\!\left(\frac{1}{2} - \mathrm{i}x\right), \qquad n \in \mathbb{Z}_+, \tag{7.2}$$

while $\varphi_{-n-1}^{\langle 1\rangle}(x) = (-1)^{n+1}\overline{\varphi_n^{\langle 1\rangle}(x)}$, $n \in \mathbb{Z}_+$.

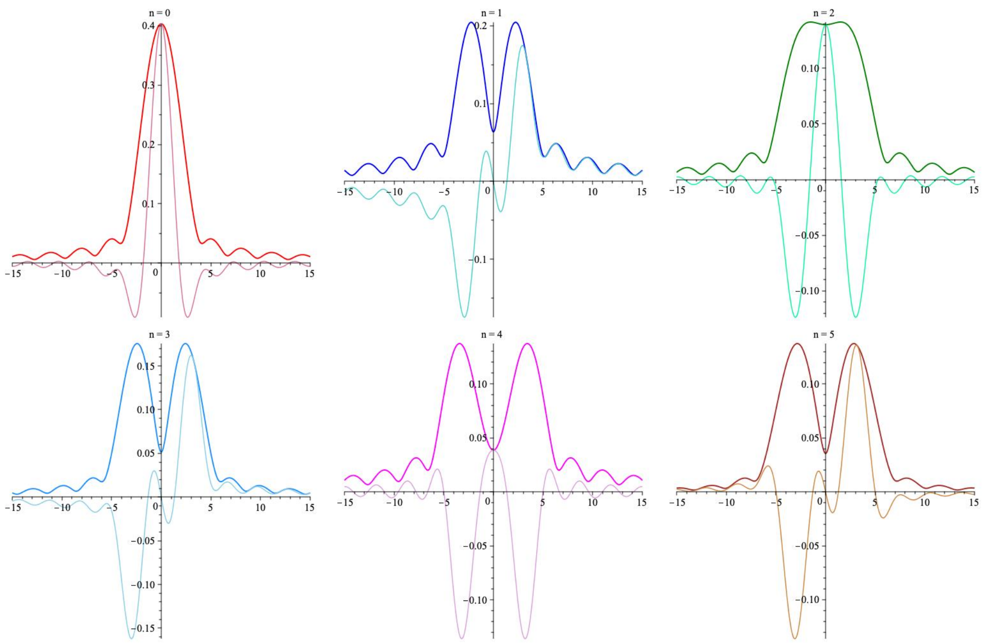

Figure 7.1: Shifted Sobolev–Hermite functions: $|\varphi_n^{\langle 1\rangle}(x,1)|$ in thicker line and darker colour and $\operatorname{Re}\varphi_n^{\langle 1\rangle}(x,1)$, for $n=0,\ldots,5$.

Proof Letting

$$\eta_n(x)=\frac{1}{\sqrt{2\pi}}\int_0^\infty \xi^n\frac{\mathrm{e}^{-\xi/2+\mathrm{i}x\xi}}{\sqrt{1+\xi^2}}\,\mathrm{d}\xi,\qquad n\in\mathbb{Z}_+,$$

we compute the generating function

$$\begin{aligned}G(x,T)=\sum_{n=0}^\infty\frac{\eta_n(x)}{n!}T^n&=\frac{1}{\sqrt{2\pi}}\int_0^\infty\frac{1}{\sqrt{1+\xi^2}}\exp\left(-\frac{\xi}{2}+T\xi+\mathrm{i}x\xi\right)\mathrm{d}\xi\\&=-\frac{\sqrt{2\pi}}{4}\left[\mathrm{Y}_0\left(\frac12-\mathrm{i}x-T\right)-\mathbf{H}_0\left(\frac12-\mathrm{i}x-T\right)\right].\end{aligned}$$

Therefore

$$\eta_n(x)=\left.\frac{\partial^n G(x,T)}{\partial T^n}\right|_{T=0}=(-1)^{n+1}\frac{\sqrt{2\pi}}{4}g^{(n)}\!\left(\frac12-\mathrm{i}x\right),\qquad n\in\mathbb{Z}_+.$$

Laguerre polynomials L_n are orthonormal and

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

(Olver et al. 2010, 18.5.12) and it follows from Theorem 1 that

$$\varphi_n^{\langle 1\rangle}(x) = \frac{\mathrm{i}^n}{\sqrt{2\pi}} \int_0^\infty \mathrm{L}_n(\xi) \frac{\mathrm{e}^{-\xi/2+\mathrm{i}x\xi}}{\sqrt{1+\xi^2}}\,\mathrm{d}\xi = \mathrm{i}^n \sum_{\ell=0}^{n} (-1)^\ell \binom{n}{\ell} \frac{\eta_\ell(x)}{\ell!},$$

thereby proving (7.2) upon the substitution of the explicit form of η_ℓ.

Extending this to $n \le -1$ is trivial. □

Corollary 1 *The functions $\varphi_n^{\langle 1\rangle}$ for $n \in \mathbb{Z}_+$ have the generating function*

$$\sum_{n=0}^{\infty} \frac{\varphi_n^{\langle 1\rangle}(x)}{n!} t^n = -\frac{\sqrt{2\pi}}{4} \mathrm{e}^{\mathrm{i}t} \sum_{\ell=0}^{\infty} \frac{(\mathrm{i}t)^\ell}{\ell!^2} g^{(\ell)}\!\left(\frac{1}{2} - \mathrm{i}x\right). \tag{7.3}$$

The proof is elementary, using (7.2). Moreover, (7.3) can be easily extended to

$$\sum_{n=-\infty}^{\infty} \frac{\varphi_n^{\langle 1\rangle}(x)}{|n|!} \zeta^n = \frac{\sqrt{2\pi}}{4} \left[\mathrm{e}^{-\mathrm{i}\zeta^{-1}} \sum_{\ell=0}^{\infty} \frac{(-\mathrm{i}\zeta^{-1})^\ell}{\ell!^2} g^{(\ell)}\!\left(\frac{1}{2}+\mathrm{i}x\right) - \mathrm{e}^{\mathrm{i}\zeta} \sum_{\ell=0}^{\infty} \frac{(\mathrm{i}\zeta)^\ell}{\ell!^2} g^{(\ell)}\!\left(\frac{1}{2}-\mathrm{i}x\right) \right],$$

which makes sense for $|\zeta| = 1$.

Since

$$z^2 \mathrm{Y}_n''(z) + z\mathrm{Y}_n'(z) + (z^2 - n^2)\mathrm{Y}_n(z) = 0,$$
$$z^2 \mathbf{H}_n''(z) + z\mathbf{H}_n'(z) + (z^2 - n^2)\mathbf{H}_n(z) = \frac{z^{n+1}}{2^{n-1}\sqrt{\pi}\Gamma(n+\frac{1}{2})}$$

(Olver et al. 2010, 11.10.5 & 11.2.7), it follows that g obeys

$$zg''(z) + g'(z) + zg(z) = -\frac{2}{\sqrt{\pi}\Gamma(\frac{1}{2})} = -\frac{2}{\pi}$$

and we can express $g^{(\ell)}$ as a linear combination of g and g' with rational coefficients. We do not pursue further this course of action. Functions $\varphi_n^{\langle s\rangle}$ for $s \ge 2$ (or even the underlying orthogonal polynomials $p_n^{\langle s\rangle}$) are no longer available in an explicit form.

7.2.2 Sobolev–Laguerre functions of the second kind

An alternative is to consider the Sobolev–Laguerre cascade of the second kind. While the orthogonal polynomials $p_n^{[s]}$ for the weight $w_s(\xi) = \mathrm{e}^{-\xi}\chi_{[0,\infty)} \sum_{\ell=0}^{s} \xi^{2\ell}$ are unknown for $s \in \mathbb{N}$, the underlying moments are trivial to compute and such polynomials can be generated at will. Also the computation of the $\varphi_n^{[s]}$s does not present a problem: for example

$$\varphi_0^{[1]}(x) = \sqrt{\frac{2}{3\pi}} \frac{1}{1-2\mathrm{i}x},$$
$$\varphi_1^{[1]}(x) = \sqrt{\frac{2}{87\pi}}\mathrm{i} \left[-\frac{4}{1-2\mathrm{i}x} + \frac{3(1+2\mathrm{i}x)}{(1-2\mathrm{i}x)^2} \right],$$

$$\varphi_2^{[1]}(x) = \sqrt{\frac{2}{16211\pi}}\mathrm{i}^2\left[\frac{34}{1-2\mathrm{i}x} - \frac{40(1+2\mathrm{i}x)}{(1-2\mathrm{i}x)^2} + \frac{29(1+2\mathrm{i}x)^2}{(1-2\mathrm{i}x)^3}\right],$$
$$\varphi_3^{[1]}(x) = \sqrt{\frac{2}{9812127\pi}}\mathrm{i}^3\left[-\frac{480}{1-2\mathrm{i}x} + \frac{762(1+2\mathrm{i}x)}{(1-2\mathrm{i}x)^2} - \frac{804(1+2\mathrm{i}x)^2}{(1-2\mathrm{i}x)^3} + \frac{559(1+2\mathrm{i}x)^3}{(1-2\mathrm{i}x)^4}\right]$$

and so on: all this seems very similar to (7.1) and for a good reason: for any $s \in \mathbb{Z}_+$ we can expand the relevant orthonormal polynomials in the Laguerre basis,

$$p_n^{[s]}(x) = \sum_{j=0}^{n} \gamma_{n,j}^{[s]} \mathrm{L}_j(x)$$

(cf. (3.5)), whereby it follows from (3.2) that

$$\varphi_n^{[s]}(x) = \sum_{j=0}^{n} \frac{\gamma_{n,j}^{[s]}}{\sqrt{2\pi}} \int_0^\infty \mathrm{L}_j(\xi)\mathrm{e}^{-\xi/2+\mathrm{i}x\xi}\,\mathrm{d}\xi = \sum_{j=0}^{n} \gamma_{n,j}^{[s]}\varphi_j^{[0]}(x).$$

Note that the matrix $\{\gamma_{n,j}^{[s]}\}_{n,j\in\mathbb{Z}_+}$ is the inverse of the banded connection matrix $C^{[s]\top}$ from Theorem 7. A similar construction applies also to $\varphi_n^{[s]}$ for $n \le -1$.

The most remarkable feature of the Malmquist–Takenaka system is that the expansion coefficients $\hat{f}_n^{[0]} = \langle f, \varphi_n^{[0]}\rangle$ can be computed for $-N+1 \le n \le N$ in $\mathcal{O}(N \log N)$ operations using the Fast Fourier Transform. By (3.7), however, once $\hat{\boldsymbol{f}}^{[0]}$ is known and assuming that the requisite derivatives of f are available, it costs just $\mathcal{O}(N)$ operations to compute

$$f_n^{[s]} = \sum_{\ell=0}^{s} \int_{-\infty}^{\infty} f^{(\ell)}(x)\overline{\varphi_n^{[s]\,(\ell)}(x)}\,\mathrm{d}x, \qquad -N+1 \le n \le N.$$

(The derivatives of $\varphi_n^{[s]}$s can be computed similarly to the functions themselves, $\boldsymbol{\varphi}_n^{[s]\,(\ell)} = C^{[s]-\top}\boldsymbol{\varphi}^{[0]\,(\ell)}$.) Altogether, the cost scales as $\mathcal{O}(sN \log N)$.

8 Conclusion

In a sequence of previous papers (Iserles & Webb 2019, Iserles & Webb 2020, Iserles & Webb 2021*b*, Iserles & Webb 2021*a*) the current authors have sketched different aspects of an overarching theory of L_2-orthonormal systems on the real line with a tridiagonal differentiation matrix. In this paper we extend the framework to orthogonality with respect to Sobolev spaces. Unlike in the case of orthogonal polynomials, where Sobolev orthogonality is of a completely different flavour to orthogonality with respect to a Borel measure (Iserles et al. 1991, Marcellán et al. 1993, Marcellán & Xu 2015), in our case we can leverage many elements of the "L_2 theory" to a Sobolev setting: the connection to standard orthogonal polynomials via a weighted Fourier transform, density in Paley–Wiener spaces and fast computation of certain expansions. Other aspects of the theory are new, in particular the existence of two cascades, the latter of which can be ascended by banded triangular connection coefficients.

The work of this paper is a stepping stone toward the development of spectral methods on the real line that respect a wide range of invariants that can be expressed as conservation of a variable-weight Sobolev norm: a couple of examples have been given in Section 1. We expect to return to this issue in a forthcoming paper.

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