On Sobolev orthogonal polynomials

Francisco Marcellán [a,*], Yuan Xu [b]

[a] *Instituto de Ciencias Matemáticas (ICMAT) and Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Spain*
[b] *Department of Mathematics, University of Oregon, Eugene OR 97403-1222, United States*

Abstract

Sobolev orthogonal polynomials have been studied extensively in the past quarter-century. The research in this field has sprawled into several directions and generates a plethora of publications. This paper contains a survey of the main developments up to now. The goal is to identify main ideas and developments in the field, which hopefully will lend a structure to the mountainous publications and help future research.
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1. Introduction

If $\langle \cdot, \cdot \rangle$ is an inner product defined on the linear space of polynomials, then orthogonal polynomials $\{p_n\}_{n \geq 0}$ with respect to the inner product are those polynomials satisfying $\langle p_n, p_m \rangle = 0$ if $n \neq m$. We call them *ordinary* orthogonal polynomials if $\langle f, g \rangle$

* Corresponding author.
 E-mail addresses: pacomarc@ing.uc3m.es (F. Marcellán), yuan@uoregon.edu (Y. Xu).

$= \int_{\mathbb{R}} f(x)g(x)d\mu$ with respect to a nonnegative Borel measure $d\mu$ supported on an infinite subset of the real line. They are called Sobolev orthogonal polynomials when the inner product involves derivatives.

Sobolev orthogonal polynomials were first considered in the early 60s of the last century. In the past 25 years, the field has seen a rapid development that leads to a large amount of publications. A rough count shows around four hundred publications in the past two decades. For a new comer, as the second author was at the beginning of this project, the size of the literature is daunting and worse still is the disarray of the literature.

The theory of ordinary orthogonal polynomials is well established and documented. One essential tool in the theory is the three-term recurrence relation that orthogonal polynomials satisfy, which holds if the multiplication operator is symmetric with respect to the inner product, that is, if $\langle xp, q \rangle = \langle p, xq \rangle$. In the Sobolev setting, however, the multiplication operator is no longer symmetric and, consequently, the three-term relation no longer holds. The deprival of this fundamental tool cannot be easily compensated. Different and ad hoc methods have been developed for dealing with different Sobolev inner products. The result is a theory of Sobolev orthogonal polynomials that appears fragmented and lack of uniformity.

The purpose of this paper is to provide an updated survey for the current state of the theory of Sobolev orthogonal polynomials. Several surveys on specific topics within the field appeared in the nineties or at the turn of the century [72,84,86,91], they were far more restrictive in their scope and need update by now. This project was initiated when the first author, who has worked extensively on the subject, led the second author, who works in several variables where Sobolev orthogonal polynomials have only been studied recently, through the literature. After intensive reading and discussion, we decided to trace the development of the subject, identify main ideas and developments, and provide some structure to the literature so that it can be more accessible for new comers and researchers interested in this field. The organization of the paper follows roughly the progress of this collective learning process, the first part of which more or less correlates with the historical development of the field.

We will limit our scope to Sobolev orthogonal polynomials with respect to those inner products that are defined by integrals with at most finite additional discrete mass points. The main Sobolev inner product that we consider can be written as

$$\langle f, g \rangle = \int_{\mathbb{R}} f(x)g(x)d\mu_0 + \sum_{k=1}^{m} \int_{\mathbb{R}} f^{(k)}(x)g^{(k)}(x)d\mu_k,$$

where $d\mu_k, k = 0, 1, \ldots, m$, are positive Borel measures on $\mathbb{R}$. There are essentially three types of such inner products in this paper:

  I. $d\mu_0, d\mu_1, \ldots, d\mu_m$ have continuous support.

 II. $d\mu_0$ has continuous support and $d\mu_1, \ldots, d\mu_m$ are supported on finite subsets.

III. $d\mu_m$ has continuous support and $d\mu_0, \ldots, d\mu_{m-1}$ are supported on finite subsets.

In the second and the third cases, we sometimes also consider mixed discrete part, for example, in the second case,

$$\langle f, g \rangle = \int_{\mathbb{R}} f(x)g(x)d\mu_0 + \left(f(0), f'(0), \ldots, f^{(m)}(0) \right) M \left(g(0), g'(0), \ldots, g^{(m)}(0) \right)^T$$

with M being an $(m+1) \times (m+1)$ matrix. We will not consider Sobolev orthogonal polynomials that involve discrete orthogonal polynomials, q-orthogonal polynomials, and complex valued orthogonal polynomials, including those on the unit circle, since the survey is already long and the ideas and methods used in these settings are often parallel to those discussed in this paper.

The list of references at the end of the paper is compiled strictly according to the materials covered in the paper. It is by no means inclusive or complete. We no doubt missed many papers that should be cited and we apologize to those authors whose work we should have cited.

The paper is organized as follows. After a brief introduction of ordinary orthogonal polynomials in Section 2, we recall the history and early results of Sobolev orthogonal polynomials in Section 3. The early results wer essentially established by the method of integration by parts, which is discussed in Section 4. The topic went into a long dormant a decade after its beginning and was awakened only when the notion of coherent pair was introduced. The main idea of coherent pair and its various extensions are expounded in a lengthy Section 5. Classical orthogonal polynomials, the Jacobi, Laguerre and Hermite polynomials, play an important role in the development and they are Sobolev orthogonal polynomials themselves for appropriately defined inner products, which will be explained in Section 6. Sobolev orthogonal polynomials for the inner products of the second type, those with derivatives appear only in the point evaluations, are discussed in Section 7. In the literature they are called either Sobolev type or discrete Sobolev orthogonal polynomials. Some of these polynomials satisfy differential equations, which and other results concerning differential equations are presented in Section 8. Two important properties of Sobolev orthogonal polynomials, zeros and asymptotics, are addressed in Section 9 and Section 10, respectively. More recently, prompted partly by problems in numerical solution of partial differential equations, Sobolev orthogonal polynomials in several variables have come into being. What is known up to date in this direction is reported in Section 11. Finally, in Section 12, we discuss Fourier expansions in Sobolev orthogonal polynomials. The lack of Christoffel–Darboux formula for Sobolev orthogonal polynomials, consequence of the lack of three-term recurrence relation, deprives an important tool for studying convergence and summability of Fourier orthogonal expansions. As a consequence, except for certain inner product of the second type and some numerical experiments, the convergence of Fourier expansions in Sobolev orthogonal polynomials has not been resolved. We consider this deficiency one of the major open problems that deserves to be studied intensively. This call of action seems a fitting point to end our survey.

2. Orthogonal polynomials

In this section, we introduce notation and basic background concerning the general structure of orthogonal polynomials. Although the results in this section are mostly classical, it is necessary to fix notations and recall results that will be essential in our discussion.

2.1. General properties of orthogonal polynomials

All functions encounter in this paper are real valued. Let Π denote the linear space of polynomials with real coefficients on the real line and, for $n = 0, 1, \ldots,$ let Π_n denote the linear subspace of polynomials of degree at most n.

We consider orthogonal polynomials on the real line. Let $\langle \cdot, \cdot \rangle$ be a symmetric bilinear form defined on $\Pi \times \Pi$. It is an inner product if $\langle p, p \rangle > 0$ for all nonzero polynomial $p \in \Pi$. A sequence of polynomials $\{P_n\}_{n \geq 0}$ is called orthogonal with respect to $\langle \cdot, \cdot \rangle$ if $\deg P_n = n$ and

$$\langle P_n, P_m \rangle = 0, \quad n \neq m.$$

P_n is said to be monic if $P_n(x) = x^n + a_{n,n-1}x^{n-1} + \cdots$. For $n = 0, 1, 2, \ldots,$ let

$$M_n := \begin{bmatrix} \langle 1, 1 \rangle & \langle 1, x \rangle & \cdots & \langle 1, x^n \rangle \\ \langle x, 1 \rangle & \langle x, x \rangle & \cdots & \langle x, x^n \rangle \\ \cdots & \cdots & \ddots & \cdots \\ \langle x^n, 1 \rangle & \langle x^n, x \rangle & \cdots & \langle x^n, x^n \rangle \end{bmatrix}.$$

If $\langle \cdot, \cdot \rangle$ is an inner product, then M_n is positive definite i.e. $\det M_n > 0$ for every $n \in \mathbb{N}_0$. If $\det M_n \neq 0$ for all $n \in \mathbb{N}_0$, then a sequence of monic orthogonal polynomials exists. In fact, the monic orthogonal polynomials are $P_0(x) = 1$ and, for $n \geq 1$,

$$P_n(x) = \frac{1}{\det M_{n-1}} \det \begin{bmatrix} & & & \langle 1, x^n \rangle \\ & M_{n-1} & & \langle x, x^n \rangle \\ & & & \vdots \\ & & & \langle x^{n-1}, x^n \rangle \\ \hline 1, x, \ldots, x^{n-1} & & & x^n \end{bmatrix}. \tag{2.1}$$

Let μ be a positive Borel measure supported on the real line such that all its moments, $\int_{\mathbb{R}} x^n d\mu$ with $n = 0, 1, 2, \ldots,$ are finite. For such a measure,

$$\langle f, g \rangle_{d\mu} := \int_{\mathbb{R}} f(x)g(x)d\mu$$

defines an inner product. We can define bilinear forms from linear functionals. Indeed, let $\mathcal{U} : \Pi \mapsto \mathbb{R}$ be a linear functional and denote its action on $p \in \Pi$ by $\langle \mathcal{U}, p \rangle$. Associated to $\mathcal{U}$ we define a bilinear form

$$\langle f, g \rangle := \langle \mathcal{U}, fg \rangle.$$

Definition 2.1. The linear functional $\mathcal{U}$ is called quasi-definite if $\det M_n \neq 0$ for all $n \in \mathbb{N}_0$, and it is called positive definite if $\det M_n > 0$ for all $n \in \mathbb{N}_0$.

When $\mathcal{U}$ is quasi-definite, orthogonal polynomials with respect to the bilinear form defined by $\mathcal{U}$ exist, which shall be called orthogonal polynomials with respect to $\mathcal{U}$. When $\mathcal{U}$ is positive definite, the bilinear form is an inner product given by $\langle \cdot, \cdot \rangle_{d\mu}$ for a positive Borel measure μ.

Let ∂ denote the derivative $\partial f(x) := f'(x)$ and let q be a fixed polynomial in Π. For a linear functional $\mathcal{U}$, the linear functionals $\partial \mathcal{U}$ and $q\mathcal{U}$ are defined, respectively, by

$$\langle \partial \mathcal{U}, p \rangle := -\langle \mathcal{U}, \partial p \rangle \quad \text{and} \quad \langle q\mathcal{U}, p \rangle := \langle \mathcal{U}, qp \rangle, \quad \forall p \in \Pi.$$

For $a \in \mathbb{R}$, the delta functional δ_a is defined by $\langle \delta_a, p \rangle = p(a)$ for all $p \in \Pi$.

For a quasi-definite linear functional $\mathcal{U}$, monic orthogonal polynomials $\{P_n\}_{n \geq 0}$ are characterized by the three-term recurrence relation

$$x P_n(x) = P_{n+1}(x) + b_n P_n(x) + c_n P_{n-1}(x), \quad n \geq 0$$

where $c_n \neq 0$ for $n \geq 1$. The three-term recurrence relation plays an important role in the study of ordinary orthogonal polynomials. It is equivalent, in particular, to the Christoffel–Darboux formula,

$$\sum_{k=0}^{n} \frac{P_k(x) P_k(y)}{h_k} = \frac{1}{h_n} \frac{P_{n+1}(x) P_n(y) - P_{n+1}(y) P_n(x)}{x - y},$$

where $h_k = \sqrt{\langle P_k, P_k \rangle}$. For orthogonal polynomials with respect to an inner product, the three-term relation holds if an only if $\langle \cdot, \cdot \rangle$ satisfies

$$\langle xp, q \rangle = \langle p, xq \rangle, \quad p, q \in \Pi$$

i.e. the multiplication operator is a symmetric operator with respect to the above inner product. This property, however, does not hold for Sobolev inner product in general as we will show in the sequel.

2.2. Classical orthogonal polynomials

These polynomials are associated with the following weight functions

(1) Hermite: $w(x) = e^{-x^2}$ on $(-\infty, \infty)$;
(2) Laguerre: $w_\alpha(x) = x^\alpha e^{-x}$ on $(0, \infty)$, $-\alpha \notin \mathbb{N}$;
(3) Jacobi: $w_{\alpha,\beta}(x) = (1-x)^\alpha (1+x)^\beta$ on $(-1, 1)$, $-\alpha \notin \mathbb{N}$, $-\beta \notin \mathbb{N}$, $-\alpha - \beta \notin \mathbb{N}$.

We denote the corresponding linear functional by $\mathcal{H}$, $\mathcal{L}_\alpha$, and $\mathcal{J}_{\alpha,\beta}$, respectively. These linear functionals are quasi-definite for all ranges of their parameters. Moreover, $\mathcal{H}$ is positive definite, $\mathcal{L}_\alpha$ is positive definite if $\alpha > -1$ and $\mathcal{J}_{\alpha,\beta}$ is positive definite if $\alpha > -1$ and $\beta > -1$.

In the positive definite case, the orthogonal polynomials for these weight functions are called classical. They are the Hermite polynomials H_n, the Laguerre polynomials $L_n^{(\alpha)}$, and the Jacobi polynomials $P_n^{(\alpha,\beta)}$, which are defined in terms of hypergeometric functions as follows,

$$H_n(x) = (2x)^n {}_2F_0 \left(\begin{array}{c} -\dfrac{n}{2}, -\dfrac{n+1}{2} \\ - \end{array}; -\dfrac{1}{x^2} \right),$$

$$L_n^{(\alpha)}(x) = \frac{(\alpha+1)_n}{n!} {}_1F_1 \left(\begin{array}{c} -n \\ \alpha+1 \end{array}; x \right),$$

$$P_n^{(\alpha,\beta)}(x) = \frac{(\alpha+1)_n}{n!} {}_2F_1\left(\begin{matrix} -n, n+\alpha+\beta+1 \\ \alpha+1 \end{matrix}; \frac{1-x}{2}\right).$$

The Gegenbauer polynomial C_n^λ is a constant multiple of the Jacobi polynomial when $\alpha = \beta = \lambda - 1/2$

$$C_n^\lambda(x) = \frac{(2\lambda)_n}{(\lambda+\frac{1}{2})_n} P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x), \quad \lambda > -\frac{1}{2}.$$

There are several characterizations of classical orthogonal polynomials. If we consider only orthogonal polynomials with respect to a real inner product, then polynomials in each classical family are eigenfunctions of a second order linear differential operator with polynomial coefficients; moreover, up to a real linear change of variables, they are the only orthogonal polynomials that satisfy this property. Let $\mathcal{U}$ be one of the classical linear functionals. Then $\mathcal{U}$ satisfies the *Pearson equation*

$$\partial(\phi\mathcal{U}) = \psi\mathcal{U}, \qquad \deg\phi \le 2 \quad \text{and} \quad \deg\psi = 1;$$

more precisely, for $-\alpha \notin \mathbb{N}$, $-\beta \notin \mathbb{N}$, and $-\alpha - \beta \notin \mathbb{N}$,

$$\partial\mathcal{H} = -2x\mathcal{H}, \qquad \partial(x\mathcal{L}_\alpha) = (-x+\alpha+1)\mathcal{L}_\alpha,$$
$$\partial((x^2-1)\mathcal{J}_{\alpha,\beta}) = ((\alpha+\beta+2)x+\alpha-\beta)\mathcal{J}_{\alpha,\beta}.$$

Furthermore, up to a linear change of variables, the only other family of linear functionals that satisfy the Pearson equation corresponds to the Bessel polynomials, and the linear functional is defined by an integral along a curve of the complex plane surrounding the origin and complex weight

$$w_\alpha(z) = \sum_{k=0}^\infty \frac{1}{(\alpha+1)_k}(-2/z)^k,$$

where $(a)_n = a(a+1)\ldots(a+n-1), n \ge 1$, and $(a)_0 = 1$ denotes the Pochhammer symbol (see [26]).

3. History and earlier results

The starting point of the Sobolev orthogonal polynomials can be traced back to the paper [67] by Lewis, who asked the following question: Let $\alpha_0, \ldots, \alpha_p$ be monotonic, non-decreasing functions defined on $[a, b]$ and let f be a function on $[a, b]$ that satisfies certain regularity conditions. Determine a polynomial P_n of degree $\le n$ that minimizes

$$\sum_{k=0}^p \int_a^b |f^{(k)}(x) - P_n^{(k)}(x)|^2 d\alpha_k(x).$$

Lewis did not use Sobolev orthogonal polynomials and gave a formula for the reminder term of the approximation as an integral of the Peano kernel. The first paper on Sobolev orthogonal polynomials was published by Althammer [9], who attributed his motivation to Lewis's paper.

The Sobolev orthogonal polynomials considered in [9] are orthogonal with respect to the inner product

$$\langle f, g \rangle_S = \int_{-1}^{1} f(x)g(x)dx + \lambda \int_{-1}^{1} f'(x)g'(x)dx, \quad \lambda > 0. \tag{3.1}$$

These Sobolev–Legendre polynomials were systematically studied in [9]. Some of the results in [9] were simplified and further extended by Schäfke in [98]. These earlier works already demonstrated several characteristic features of Sobolev orthogonal polynomials. Let $S_n(\cdot; \lambda)$ denote the orthogonal polynomial of degree n with respect to the inner product $\langle \cdot, \cdot \rangle_S$, normalized so that $S_n(1; \lambda) = 1$, and let P_n denote the nth Legendre polynomial. The following properties hold for $S_n(\cdot; \lambda)$:

(1) $\{S_n(\cdot; \lambda)\}_{n \geq 0}$ satisfies a differential equation

$$\lambda S_n''(x; \lambda) - S_n(x; \lambda) = A_n P_{n+1}'(x) + B_n P_{n-1}'(x),$$

where A_n and B_n are constants that can be given by explicit formulas.

(2) $\{S_n(\cdot; \lambda)\}_{n \geq 0}$ satisfies a recursive relation

$$S_n(x; \lambda) - S_{n-2}(x; \lambda) = a_n(P_n(x) - P_{n-2}(x)), \quad n = 1, 2, \ldots.$$

(3) $S_n(\cdot; \lambda)$ has n real simple zeros in $(-1, 1)$.

For a more detailed account on the development of these results, we refer to the original articles or to [91], which contains a nice survey of early history of Sobolev orthogonal polynomials. The Sobolev–Legendre polynomials were also studied by Gröbner, who established a version of the Rodrigues formula for in [48], which states that, up to a constant factor c_n,

$$S_n(x; \lambda) = c_n \frac{\partial^n}{1 - \lambda \partial^2} \left((x^2 - x)^n - \alpha_n (x^2 - x)^{n-1} \right)$$

where α_n are real numbers explicitly given in terms of λ and n. Furthermore, in [25], Cohen proved that the zeros of $S_n(\cdot; \lambda)$ interlace with those of the Legendre polynomial P_{n-1} if $\lambda \geq 2/n$, and he also established the sign of the connecting coefficients of $S_n(\cdot; \lambda)$ expanded in terms of the sequence $\{S_m(\cdot; \mu)\}_{m \geq 0}$ for $\lambda \neq \mu$.

In [9], Althammer also gave an example in which he replaced dx in the second integral in $\langle \cdot, \cdot \rangle_S$ by $w(x)dx$ with $w(x) = 10$ for $-1 \leq x < 0$ and $w(x) = 1$ for $0 \leq x \leq 1$, and made the observation that $S_2(x; \lambda)$ for this new inner product has one real zero outside of $(-1, 1)$.

Another earlier paper is [20], in which Brenner considered the inner product

$$\langle f, g \rangle := \int_0^\infty f(x)g(x)e^{-x}dx + \lambda \int_0^\infty f'(x)g'(x)e^{-x}dx, \quad \lambda > 0,$$

and obtained results similar to those of Althammer.

An important paper in the early development of the Sobolev orthogonal polynomials is [99], in which Schäfke and Wolf considered a family of inner products

$$\langle f, g \rangle_S = \sum_{j,k=0}^\infty \int_a^b f^{(j)}(x)g^{(k)}(x)v_{j,k}(x)w(x)dx, \tag{3.2}$$

where w and (a, b) are one of the three classical cases, Hermite, Laguerre and Jacobi, and the functions $v_{j,k}$ are polynomials that satisfy $v_{j,k} = v_{k,j}$, $j, k = 0, 1, 2, \ldots$, and permit writing the inner product (3.2) as

$$\langle f, g \rangle_S = \int_a^b f(x) \mathcal{B} g(x) w(x) dx \quad \text{with } \mathcal{B} g := w^{-1} \sum_{j,k=0}^{\infty} (-1)^j \partial^j (w v_{j,k} \partial^k) g \quad (3.3)$$

through integration by parts. Under further restrictions on $v_{j,k}$, they narrowed down to eight classes of Sobolev orthogonal polynomials, which they call simple generalization of classical orthogonal polynomials. These cases are given by

A1. $v_{j,k} = 0$, with $|j - k| > 1$, $v_{j,j} = (1 - x^2)^j (b_j x + c_j)$, $v_{j,j-1} = d_j (1 - x^2)^j$.

A2. $v_{j,k} = 0$, with $|j - k| > 2$, $v_{j,j} = (1 - x^2)^j (b_j (1 - x^2) + c_j)$, $v_{j,j-1} = d_j x (1 - x^2)^j$, $j \geq 1$, $v_{j,j-2} = e_j (1 - x^2)^j$, $j \geq 2$.

A3. $v_{j,k} = 0$, with $|j - k| > 1$, $v_{0,0} = c_0$, $v_{j,j} = (1 + x)^j (1 - x)^{j-1} (b_j x + c_j)$, $v_{j,j-1} = d_j (1 + x)^j (1 - x)^{j-1}$, $j \geq 1$.

A4. $v_{j,k} = 0$, with $|j - k| > 2$, $v_{0,0} = c_0$, $v_{j,j} = (1 - x^2)^{j-1} (b_j (1 - x^2) + c_j)$, $v_{j,j-1} = d_j x (1 - x^2)^{j-1}$, $j \geq 1$, $v_{j,j-2} = e_j (1 - x^2)^{j-1}$, $j \geq 2$.

B1. $v_{j,k} = 0$, with $|j - k| > 1$, $v_{j,j} = x^j (b_j x + c_j)$, $v_{j,j-1} = d_j x^j$.

B2. $v_{j,k} = 0$, with $|j - k| > 1$, $v_{0,0} = c_0$, $v_{j,j} = x^{j-1} (b_j x + c_j)$, $v_{j,j-1} = d_j x^{j-1}$, $j \geq 1$.

C1. $v_{j,k} = 0$, with $|j - k| > 1$, $v_{j,j} = b_j x + c_j$, $v_{j,j-1} = d_j$.

C2. $v_{j,k} = 0$, with $|j - k| > 2$, $v_{j,j} = b_j x^2 + c_j$, $v_{j,j-1} = d_j x$, $j \geq 1$, $v_{j,j-2} = e_j$,

where the real constants b_j, c_j, d_j, and e_j are subject to additional conditions for the positive-definiteness of (3.2) and so that formula (3.3) is true. The main results in [99] extended all earlier results on Sobolev orthogonal polynomials. Let $\{S_n\}_{n \geq 0}$ denote a sequence of Sobolev orthogonal polynomials with respect to $\langle \cdot, \cdot \rangle_S$ in (3.2) and let $\{T_n\}_{n \geq 0}$ denote a sequence of ordinary orthogonal polynomials with respect to the inner product

$$\langle f, g \rangle = \int_a^b f(x) g(x) u(x) w(x) dx,$$

where u is a polynomial of degree at most 2, which is known explicitly in each class. It was shown in [99] that, under appropriate normalizations of S_n and T_n, there exists a sequence of real numbers $\{a_n\}_{n \geq 0}$ such that

$$S_{n+r} - S_n = a_{n+r} u T_{n+r-k},$$

where $r = 1$ or r depending on the case, k equals the degree of u and a_{n+r} is a constant, and the differential operator $\mathcal{B}$ satisfies

$$\mathcal{B} S_n = b_n (a_n T_{n+s} - a_{n+r} T_{n+s-r}),$$

where $s = 0$, 1, or 2, depending on the class. Furthermore, sufficient conditions were given in [99] for S_n to have all simple zeros in (a, b). The paper, however, is not easy to digest.

Except the theorem on zeros, results were not stated in theorems and it is no small task to figure out the exact statement for each individual class.

The primary tool in the early study of Sobolev orthogonal polynomials is integration by parts. Schäfke and Wolf explored when this tool is applicable and outlined potential Sobolev inner products. It is remarkable that their work appeared in such an early stage of the development of Sobolev orthogonal polynomials. However, instead of stirred to action by [99], the study of Sobolev orthogonal polynomials unexpectedly became largely dormant for nearly two decades, from which it reemerged only when a new ingredient, *coherent pairs*, was introduced by Iserles, Koch, Nørsett and Sanz-Serna in [54].

4. Method of integration by parts

In this section, we explain the method of integration by parts in the study of Sobolev orthogonal polynomials by considering the inner product that involves only first order derivative,

$$\langle f, g \rangle_S := \langle f, g \rangle + \lambda \langle f', g' \rangle \quad \text{with } \langle f, g \rangle := \int_a^b f(x) g(x) d\mu(x), \tag{4.1}$$

where we assume that $d\mu = u(x)dx$ and u satisfies the relation

$$\partial(\phi(x)u(x)) = \psi(x)u(x), \tag{4.2}$$

in which ϕ and ψ are fixed polynomials, with ϕ monic and $\deg \psi \geq 1$, and we assume that ϕ or u vanish on the end points of the interval (a, b), under limit if $a = -\infty$ or $b = \infty$, so that integration by parts can be carried out.

In the case of the Laguerre weight function $w_\alpha(x) = x^\alpha e^{-x}$, $\phi(x) = x$ and $\psi(x) = \alpha + 1 - x$. In the case of the Gegenbauer weight function $w_\lambda(x) = (1-x^2)^{\lambda-\frac{1}{2}}$, $\phi(x) = (1-x^2)$ and $\psi(x) = -(2\lambda + 1)x$.

Associated with the inner product (4.1), the following differential operator is useful,

$$\mathcal{F} := \phi(x)I - \lambda \mathcal{F}_0, \quad \mathcal{F}_0 := [u(x)]^{-1}\phi(x)\partial [u(x)\partial],$$

where I denotes the identity operator. Applying (4.2) allows us to write $\mathcal{F}_0$ as

$$\mathcal{F}_0 = \phi(x)\partial^2 + [\psi(x) - \phi'(x)]\partial.$$

Proposition 4.1. *Assume that $u(x)\mathcal{F}_0$ is zero when $x = a$ and $x = b$. Then, for $f, g \in \Pi$,*
(1) $\langle \phi f, g \rangle_S = \langle f, \mathcal{F}g \rangle$.
(2) $\mathcal{F}$ *is self-adjoint; that is,* $\langle \mathcal{F}f, g \rangle_S = \langle f, \mathcal{F}g \rangle_S$.

Proof. Integration by parts shows immediately that $\langle (\phi f)', g' \rangle = -\langle \phi f, \mathcal{F}_0 g \rangle$, from which (1) follows readily. Furthermore, it shows that

$$\langle (\mathcal{F}_0 f)', g' \rangle = -\int_a^b \mathcal{F}_0 f(x)(g'(x)u(x))'dx$$

$$= -\int_a^b (f'(x)u(x))' \mathcal{F}_0 g(x)dx = \langle f', (\mathcal{F}_0 g)' \rangle,$$

where the integration by parts is justified since $u(x)\mathcal{F}_0$ is zero when $x = a$ or $x = b$, which can then be used to verify (2). $\quad \square$

Let again $\{S_n(\cdot; \lambda)\}_{n \geq 0}$ be the sequence of monic Sobolev polynomials and let $\{P_n\}_{n \geq 0}$ be the sequence of monic polynomials orthogonal with respect to $\langle \cdot, \cdot \rangle$.

Proposition 4.2. *Assume that ϕ is of degree s and ψ is of degree at most $s - 1$. Then, for $n \geq s$,*

(i) $\phi(x)P_n(x, d\mu) = S_{n+s}(x; \lambda) + \sum_{j=n-s}^{n+s-1} a_{j,n}(\lambda)S_{n+j}(x; \lambda)$,

(ii) $\mathcal{F}S_n(x; \lambda) = S_{n+s}(x; \lambda) + \sum_{j=n-s}^{n+s-1} b_{j,n}(\lambda)S_{n+j}(x; \lambda)$.

Proof. The additional assumptions on ϕ and ψ show that $\mathcal{F}_0 : \Pi_n \mapsto \Pi_{n+s-2}$, so that $\mathcal{F} : \Pi_n \to \Pi_{n+s}$. By (1) of the previous proposition, $\langle \phi P_n(\cdot; d\mu), g \rangle_S = \langle P_n(\cdot; d\mu), \mathcal{F}g \rangle = 0$ either if $\mathcal{F}g \in \Pi_{n-1}$ or if $g \in \Pi_{n-s-1}$, which implies (i). The same argument proves (ii) as well. $\quad \square$

The relation in (i) is the recursive relation and (ii) is the difference–differential equation satisfied by the Sobolev orthogonal polynomials. The constants $a_{j,n}$ and $b_{j,n}$ can be explicitly determined in the case of the classical Laguerre weight w_α and the Gegenbauer weight w_λ.

Take the Laguerre weight w_α as an example. The monic Laguerre polynomial of degree n is $P_n(x) := n!(-1)^n L_n^{(\alpha)}(x)$. By the property of the Laguerre polynomial and its derivative, we have

$$Q_n'(x) = nP_{n-1}(x), \quad \text{where } Q_n(x) := P_n(x) + nP_{n-1}(x). \tag{4.3}$$

It follows readily that $\langle Q_n, q \rangle_S = 0$ if $q \in \Pi_{n-2}$, which implies immediately that

$$Q_n(x) = S_n(x; \lambda) + d_{n-1}(\lambda)S_{n-1}(x; \lambda) \tag{4.4}$$

for some constant $d_{n-1}(\lambda)$. Both the differential relation and the recursive relation in Proposition 4.2 can be made explicit using the constant $d_n(\lambda)$. For example, using the three-term relation for the monic Laguerre polynomial and (4.4), the recurrence relation (i) becomes

$$xP_n(x) = S_{n+1}(x; \lambda) + [n + \alpha + d_n(\lambda)]S_n(x; \lambda) + [(n + \alpha)d_{n-1}(\lambda)]S_{n-1}(\lambda; x).$$

Finally, the value of $d_{n-1}(\lambda)$ can be deduced recursively.

Proposition 4.3. *For $n = 2, 3, \ldots,$*

$$d_n(\lambda) = \frac{(n + 1)(n + \alpha)}{(\lambda + 2)n + \alpha - d_{n-1}(\lambda)} \quad \text{with } d_1(\lambda) := \frac{2(\alpha + 1)}{\lambda + \alpha + 1}.$$

Proof. Using the relation (4.4) for both $S_{n+1}(\cdot; \lambda)$ and $S_n(\cdot; \lambda)$, it follows that

$$0 = \langle S_{n+1}, S_n \rangle_S = \langle Q_{n+1}, Q_n \rangle_S - d_n(\lambda)\langle Q_n, Q_n \rangle_S + d_n(\lambda)d_{n-1}(\lambda)\langle Q_{n-1}, Q_n \rangle_S.$$

Evaluating the inner products in the right hand side by using (4.3), this gives the stated recursive relation. $\quad \square$

The recurrence relation shows that $d_n(\lambda)$ is a rational function of λ. In particular, if we express it as $d_n(\lambda) = (n + 1)(n + \lambda)q_{n-1}(\lambda)/q_n(\lambda)$, then $q_n(\lambda)$ satisfies a three-term recurrence relation and $q_n(\lambda)$ is related to the Pollaczek polynomials.

The monic Gegenbauer polynomial $P_n^\lambda(x)$ satisfies the relation

$$P_n^\lambda(x) = \frac{1}{n+1} \frac{d}{dx} P_{n+1}^\lambda(x) - \frac{\lambda - 1}{4(n + \lambda - 1)(n + \lambda)} \frac{d}{dx} P_{n-1}^\lambda(x).$$

Using the parity of the Gegenbauer polynomials, the above procedure for the Laguerre weight can be carried out for the Sobolev orthogonal polynomials associated with the Gegenbauer weight w_λ.

The above analysis shows how the classical work of Althammer for the Legendre weight and Brenner for e^{-x}, the Laguerre weight with $\alpha = 0$, can be worked out. This streamlined analysis was carried out in [77,78], which already incorporated the idea of the coherent pair that will be addressed in the next section. The method of integration by parts is applicable to Sobolev inner products involving derivatives of higher order, which gives an indication how the general setting of Schäfke and Wolf in [99] can be developed. It is no longer clear, however, if the finer results that hold for the Laguerre and the Gegenbauer weights can be established in the general setting of [99].

5. Coherent pairs

The notion of coherent pair was first introduced in [54] and it has become an important tool and a source of new development. Its appearance coincides with the revival of the field of Sobolev orthogonal polynomials, which has flourished ever since. This section explains this notion and its various generalizations.

5.1. Coherent pairs

The coherent pair introduced in [54] is defined for the inner product

$$\langle f, g \rangle_\lambda = \int_a^b f(x)g(x)d\mu_0(x) + \lambda \int_a^b f'(x)g'(x)d\mu_1(x), \tag{5.1}$$

where $-\infty \le a < b \le \infty$, μ_0 and μ_1 are positive Borel measures on the real line with finite moments of all orders. Let $P_n(\cdot; d\mu_i)$ denote the monic orthogonal polynomial of degree n with respect to $d\mu_i$.

Definition 5.1. The pair $\{d\mu_0, d\mu_1\}$ is called coherent if there exists a sequence of nonzero real numbers $\{a_n\}_{n \ge 1}$ such that

$$P_n(\cdot; d\mu_1) = \frac{P_{n+1}'(\cdot; d\mu_0)}{n+1} + a_n \frac{P_n'(\cdot; d\mu_0)}{n}, \quad n \ge 1. \tag{5.2}$$

If $[a, b] = [-c, c]$ and $d\mu_0$ and $d\mu_1$ are both even, then $\{d\mu_0, d\mu_1\}$ is called a symmetrically coherent pair if

$$P_n(\cdot; d\mu_1) = \frac{P_{n+1}'(\cdot; d\mu_0)}{n+1} + a_n \frac{P_{n-1}'(\cdot; d\mu_0)}{n-1}, \quad n \ge 2. \tag{5.3}$$

In the case of $d\mu_1 = d\mu_0$, we call $d\mu_0$ self-coherent.

For the classical orthogonal polynomials, it is easy to see that the following examples are coherent pairs:

Example 5.2. The Laguerre measure $d\mu = x^\alpha e^{-x} dx, \alpha > -1$, is an example of a self-coherent pair. The Gegenbauer measure $d\lambda = (1 - x^2)^{\lambda-1/2}, \lambda > 0$, is an example of a symmetrically self-coherent pair. The Jacobi weight yields a natural coherent pair; for $\alpha, \beta > -1$

$$d\mu_0 = (1 - x)^\alpha (1 + x)^\beta \quad \text{and} \quad d\mu_1 = (1 - x)^{1+\alpha}(1 + x)^{1+\beta}.$$

Let $\{S_n(\cdot; \lambda)\}_{n\geq 0}$ denote the sequence of monic Sobolev orthogonal polynomials with respect to $\langle \cdot, \cdot \rangle_\lambda$. Then $S_n(\cdot; \lambda)$ is given by the determinant expression (2.1). It is easy to see that

$$\Lambda_n(x) := \lim_{\lambda \to \infty} S_n(x; \lambda)$$

defines a monic polynomial $\Lambda_n(x)$ of degree n which satisfies the following properties

$$\Lambda'_n(x) = n P_{n-1}(x; d\mu_1) \quad \text{and} \quad \int_{\mathbb{R}} \Lambda_n(x) d\mu_0 = 0, \quad n \geq 1. \tag{5.4}$$

Theorem 5.3. *If $\{d\mu_0, d\mu_1\}$ is a coherent pair, then*

$$S_n(x; \lambda) + b_{n-1}(\lambda) S_{n-1}(x; \lambda) = P_n(x; d\mu_0) + \widehat{a}_{n-1} P_{n-1}(x; d\mu_0), \tag{5.5}$$

where $\widehat{a}_{n-1} = n a_n/(n - 1)$ and $b_{n-1}(\lambda) = \widehat{a}_{n-1} \|P_{n-1}(\cdot; d\mu_0)\|^2_{d\mu_0} / \|S_{n-1}(\cdot; \lambda)\|^2_\lambda$.

Proof. By (5.2) and (5.4), we see that

$$\Lambda_n(x) = P_n(x; d\mu_0) + \widehat{a}_{n-1} P_{n-1}(x; d\mu_0). \tag{5.6}$$

For $0 \leq j \leq n - 2$, it follows from (5.4) that

$$\langle \Lambda_n, S_j(\cdot; \lambda) \rangle_\lambda = \langle \Lambda_n, S_j(\cdot; \lambda) \rangle_{d\mu_0} + n\langle P_{n-1}(\cdot; d\mu_1) S'_j(\cdot; \lambda) \rangle_{d\mu_1} = 0,$$

which implies, considering the expansion of Λ_n in $S_j(\cdot; \lambda)$, that

$$\Lambda_n(x) = S_n(x; \lambda) + b_{n-1}(\lambda) S_{n-1}(x; \lambda), \quad \text{where } b_{n-1}(\lambda) = \frac{\langle \Lambda_n, S_{n-1}(\cdot; \lambda) \rangle_\lambda}{\|S_{n-1}(\cdot; \lambda)\|^2_\lambda}.$$

The formula of $b_{n-1}(\lambda)$ follows from $\langle \Lambda'_n, S'_{n-1}(\cdot; \lambda) \rangle_{d\mu_1} = 0$ as well as from the fact that both $P_{n-1}(\cdot; d\mu_0)$ and $S_{n-1}(\cdot; \lambda)$ are monic. $\square$

Since $b_{n-1}(\lambda)$ depends only on $S_{n-1}(\cdot; \lambda)$, the identity (5.5) can be used to compute $S_n(\cdot; \lambda)$ inductively. Furthermore, it implies the expansion

$$S_n(x; \lambda) = P_n(x; d\mu_0) + \sum_{k=0}^{n-1} \Big(\prod_{j=k+1}^{n-1} b_j(\lambda) \Big)(\widehat{a}_k - b_k(\lambda)) P_k(x; d\mu_0),$$

where we adopt the convention that $\prod_{j=n}^{n-1} b_j(\lambda) = 1$.

In [54], a different normalization of Sobolev orthogonal polynomials is chosen. Let $P_n = P_n(\cdot; d\mu_0)$. Define

$$\widetilde{S}_n(x;\lambda) := \frac{1}{\prod_{k=1}^{n-1} \|P_k\|_{d\mu_0}^2} \det \begin{bmatrix} \langle P_1, P_1 \rangle_\lambda & \langle P_1, P_2 \rangle_\lambda & \ldots & \langle P_1, P_n \rangle_\lambda \\ \langle P_2, P_1 \rangle_\lambda & \langle P_2, P_2 \rangle_\lambda & \ldots & \langle P_2, P_n \rangle_\lambda \\ \ldots & \ldots & \ddots & \ldots \\ \langle P_{n-1}, P_1 \rangle_\lambda & \langle P_{n-1}, P_2 \rangle_\lambda & \ldots & \langle P_{n-1}, P_n \rangle_\lambda \\ P_1(x) & P_2(x) & \ldots & P_n(x) \end{bmatrix}.$$

With this normalization, the identity (5.5) becomes

$$\widetilde{S}_n(x;\lambda) - \widetilde{S}_{n-1}(x;\lambda) = a_n(\lambda)(P_n(x; d\mu_0) - P_{n-1}(x; d\mu_0))$$

and the coefficients $\alpha_k(\lambda)$ in the expansion

$$\widetilde{S}_n(x;\lambda) = \sum_{k=1}^{n-1} \alpha_k(\lambda) P_k(x; d\mu_0) + a_n(\lambda) P_n(x; d\mu_0)$$

depend only on k. Moreover, $\alpha_k(\lambda)$ is a polynomial of degree k in the variable λ such that $\alpha_k(0) = 0$. Furthermore, let $R_k(\lambda) := \alpha_{k+1}(\lambda)/\lambda$; then the sequence of polynomials $\{R_k\}_{k \geq 0}$, for which $\deg R_k = k$, satisfies a three-term relation and, as a consequence, is a sequence of orthogonal polynomials with respect to a positive Borel measure. In the case of the Laguerre weight $d\mu_0(x) = d\mu_1(x) = x^\alpha e^{-x} dx$ on $[0, \infty)$, the $R_k(\lambda)$ are, up to a multiple constant, Pollaczek polynomials.

In [89], it was observed that the zeros of Λ_n interlace with those of $P_{n-1}(\cdot; d\mu_0)$ and with those of $P_n(\cdot; d\mu_0)$. Consequently, if λ is large enough, then $S_n(\cdot; \lambda)$ has n simple, real zeros that interlace with the zeros of $P_{n-1}(\cdot; d\mu_0)$ and with those of $P_{n-1}(\cdot; d\mu_1)$.

Using (5.5) and the three-term relation for $P_n(\cdot; d\mu_0)$, it is possible to derive a recurrence relation for $\{S_n(\cdot; \lambda)\}$, as observed in [29]. When $\{\Lambda_n\}_{n \geq 0}$ is a sequence of orthogonal polynomials, which holds, by (5.4), if $d\mu_1$ is classical, the recurrence relation is just the three-term recurrence relation of $\{\Lambda_n\}_{n \geq 0}$ written in $S_n(\cdot; \lambda)$ by (5.6).

5.2. Determination of coherent pairs

Because of their applications in Sobolev orthogonal polynomials, an immediate question is to identify all coherent pairs. For this purpose, the more general notion of orthogonality in terms of linear functionals is often considered. The notion of coherent pair can be extended to the linear functionals $\{\mathcal{U}_0, \mathcal{U}_1\}$, if the relation (5.2) holds with $P_n(\cdot; d\mu_i)$ replaced by $P_n(\cdot; \mathcal{U}_i)$. For classical orthogonal polynomials, we allow the parameters in $\mathcal{L}^{(\alpha)}$ and $\mathcal{J}^{(\alpha, \beta)}$ to be negative real numbers but not negative integers.

The first step of identifying all coherent pairs was taken in [79], where the coherent pairs were identified when either $\mathcal{U}_0$ or $\mathcal{U}_1$ is classical in the extended sense. Since the derivative of a classical orthogonal polynomial is again a classical orthogonal polynomial (with different parameter), (5.2) reduces to

$$Q_n = P_n + c_n P_{n-1}, \quad n \geq 1,$$

where either $\{Q_n\}_{n \geq 0}$ or $\{P_n\}_{\geq 0}$ is a sequence of classical orthogonal polynomials. Comparing the coefficients of the three-term relations satisfied by $\{Q_n\}_{n \geq 0}$ and $\{P_n\}_{n \geq 0}$ in the above identity, all coherent pairs when one of the measures is classical in the extended sense were found in [79].

The next important step is [77], which shows that if $\{\mathcal{U}_0, \mathcal{U}_1\}$ is a coherent pair, then

$$n\frac{P_n(x; \mathcal{U}_0)}{\|P_n(\cdot; \mathcal{U}_0)\|_{\mathcal{U}_0}^2}\mathcal{U}_0 = \partial(Q_n\mathcal{U}_1), \quad n \geq 1, \tag{5.7}$$

where, with a_n being the coefficient in (5.2),

$$Q_n(x) := a_n\frac{P_n(x; \mathcal{U}_1)}{\|P_n(\cdot; \mathcal{U}_1)\|_{\mathcal{U}_1}^2} - \frac{P_{n-1}(x; \mathcal{U}_1)}{\|P_{n-1}(\cdot; \mathcal{U}_0)\|_{\mathcal{U}_0}^2}.$$

The final step at identifying all coherent pairs was taken in [92], where the following theorem was established.

Theorem 5.4. *If $\{\mathcal{U}_0, \mathcal{U}_1\}$ is a coherent pair, then at least one of them has to be classical in the extended sense.*

The proof in [92] started with the observation that the relation (5.7) with $n = 1$ and $n = 2$ implies the existence of polynomials ϕ of degree at most 3, χ of degree at most 2 and ψ of degree exactly 2, such that

$$\phi\partial\mathcal{U}_1 = \chi\mathcal{U}_1, \qquad \phi\mathcal{U}_0 = \psi\mathcal{U}_1, \qquad \chi\mathcal{U}_0 = \psi\partial\mathcal{U}_1, \tag{5.8}$$

where ϕ, χ and ψ can be given explicitly in terms of $P_1(\cdot; \mathcal{U}_0)$, $P_2(\cdot; \mathcal{U}_0)$, Q_1 and Q_2. In particular, $\psi = Q_1 Q_2' - Q_1' Q_2$. The polynomial ψ has two zeros. If the two zeros coincide at the point ξ, then $\psi'(\xi) = 0$ and, as a result, $Q_1(\xi) = 0$, which can be used to show that $\phi(\xi) = 0$. Writing $\phi(x) = (x - \xi)\tilde{\phi}(x)$, it can then be shown, by eliminating $\partial\mathcal{U}_1$ in (5.8), that $\tilde{\phi}_0\mathcal{U}_0 = c(x - \xi)\mathcal{U}_1$, where c is a constant, from which it follows that $\mathcal{U}_0$ satisfies the Pearson equation $\partial(\tilde{\phi}\mathcal{U}_0) = \eta\mathcal{U}_0$, where η is a polynomial of degree 1. As the solution of the Pearson equation, $\mathcal{U}_0$ has to be classical. When the two zeros of ψ are different, $\mathcal{U}_1$ can be shown to be classical; the analysis in this case, however, is more involved.

Together, [79,92] give a complete list of coherent pairs. In the case of $\mathcal{U}_0$ and $\mathcal{U}_1$ are positive definite linear functionals associated with measures $d\mu_0$ and $d\mu_1$, these cases are given as follows:

Laguerre case

(1) $d\mu_0(x) = (x - \xi)x^{\alpha-1}e^{-x}dx$ and $d\mu_1(x) = x^\alpha e^{-x}dx$, where if $\xi < 0$ then $\alpha > 0$, and if $\xi = 0$ then $\alpha > -1$.
(2) $d\mu_0(x) = x^\alpha e^{-x}dx$ and $d\mu_1(x) = \frac{x^{\alpha+1}e^{-x}}{x-\xi}dx + M\delta_\xi$, where if $\xi < 0, \alpha > -1$ and $M \geq 0$.
(3) $d\mu_0(x) = e^{-x}dx + M\delta_0$ and $d\mu_1(x) = e^{-x}dx$, where $M \geq 0$.

Jacobi case

(1) $d\mu_0(x) = |x - \xi|(1-x)^{\alpha-1}(1+x)^{\beta-1}dx$ and $d\mu_1(x) = (1-x)^\alpha(1+x)^\beta dx$, where if $|\xi| > 1$ then $\alpha > 0$ and $\beta > 0$, if $\xi = 1$ then $\alpha > -1$ and $\beta > 0$, and if $\xi = -1$ then $\alpha > 0$ and $\beta > -1$.
(2) $d\mu_0(x) = (1-x)^\alpha(1+x)^\beta dx$ and $d\mu_1(x) = \frac{1}{|x-\xi|}(1-x)^{\alpha+1}(1+x)^{\beta+1}dx + M\delta_\xi$, where $|\xi| > 1, \alpha > -1$ and $\beta > -1$, and $M \geq 0$.
(3) $d\mu_0(x) = (1+x)^{\beta-1}dx + M\delta_1$ and $d\mu_1(x) = (1+x)^\beta dx$, where $\beta > 0$ and $M \geq 0$.
(4) $d\mu_0(x) = (1-x)^{\alpha-1}dx + M\delta_{-1}$ and $d\mu_1(x) = (1-x)^\alpha dx$, where $\alpha > 0$ and $M \geq 0$.

The similar analysis was also carried out for symmetrically coherent pairs in the work cited above. They lead to the following list of symmetrically coherent pairs.

Hermite case

(1) $d\mu_0(x) = e^{-x^2}dx$ and $d\mu_1(x) = \frac{1}{x^2+\xi^2}e^{-x^2}dx$, where $\xi \neq 0$.

(2) $d\mu_0(x) = (x^2 + \xi^2)e^{-x^2}dx$ and $d\mu_1(x) = e^{-x^2}dx$, where $\xi \neq 0$.

Gegenbauer case

(1) $d\mu_0(x) = (1 - x^2)^{\alpha-1}dx$ and $d\mu_1(x) = \frac{1}{x^2+\xi^2}(1 - x^2)^{\alpha}dx$, where $\xi \neq 0$ and $\alpha > 0$.

(2) $d\mu_0(x) = (1 - x^2)^{\alpha-1}dx$ and $d\mu_1(x) = \frac{1}{\xi^2-x^2}(1 - x^2)^{\alpha}dx + M\delta_{\xi} + M\delta_{-\xi}$, where $|\xi| \geq 1$, $\alpha > 0$ and $M \geq 0$.

(3) $d\mu_0(x) = (x^2 + \xi^2)(1 - x^2)^{\alpha-1}dx$ and $d\mu_1(x) = (1 - x^2)^{\alpha}dx$, where $\alpha > 0$.

(4) $d\mu_0(x) = (\xi^2 - x^2)(1 - x^2)^{\alpha-1}dx$ and $d\mu_1(x) = (1 - x^2)^{\alpha}dx$, where $|\xi| \geq 1$ and $\alpha > 0$.

(5) $d\mu_0(x) = dx + M\delta_1 + M\delta_{-1}$ and $d\mu_1(x) = dx$, where $M \geq 0$.

5.3. Generalized coherent pairs

We deduced the identity (5.5) from the definition (5.2) of the coherent pair. In the reverse direction, however, (5.2) does not follow from the identity (5.5), as observed in [56]. We restate (5.5) below,

$$S_n(x; \lambda) + b_{n-1}(\lambda)S_{n-1}(x; \lambda) = P_n(x; d\mu_0) + \widehat{a}_{n-1}P_{n-1}(x; d\mu_0), \quad n \geq 1. \quad (5.5')$$

For convenience, we let $\mathsf{S}_n(x)$ denote the left hand side of (5.5'). Clearly S'_n can be expanded in terms of $\{P_k(\cdot; d\mu_1)\}$,

$$\mathsf{S}'_n(x) = nP_{n-1}(x; d\mu_1) + \sum_{k=0}^{n-2} d_{k,n}P_k(x; d\mu_1), \quad d_{k,n} = \frac{\langle \mathsf{S}'_n, P_k(\cdot; d\mu_1)\rangle_{d\mu_1}}{\|P_k(\cdot; d\mu_1)\|^2_{d\mu_1}}.$$

For $0 \leq j \leq n - 2$, it follows directly from the definition of S_n that $\langle \mathsf{S}_n, P_j(\cdot; d\mu_1)\rangle_{\lambda} = 0$ and it follows from (5.5) that $\langle \mathsf{S}_n, P_j(\cdot; d\mu_1)\rangle_{d\mu_0} = 0$. Consequently, by the definition of $\langle \cdot; \cdot \rangle_{\lambda}$, we must have $\langle \mathsf{S}'_n, P_j(\cdot; d\mu_1)\rangle_{d\mu_1} = 0$ for $0 \leq j \leq n - 2$, which implies that $d_{k,n} = 0$ if $0 \leq k \leq n - 2$. Hence,

$$\mathsf{S}'_n(x) = P'_n(x; d\mu_0) + \widehat{a}_{n-1}P'_{n-1}(x; d\mu_0)$$
$$= nP_{n-1}(x; d\mu_1) + d_{n-2,n}P_{n-2}(x; d\mu_1).$$

Recall that $\widehat{a}_n = (n + 1)a_n/n$. Setting $b_{n-2} = d_{n-2,n}/n$ and shifting the index from n to $n + 1$, we conclude the following relation between $\{P_n(\cdot; d\mu_0)\}$ and $\{P_n(\cdot; d\mu_1)\}$,

$$P_n(x; d\mu_1) + b_{n-1}P_{n-1}(x; d\mu_1) = \frac{P'_{n+1}(x; d\mu_0)}{n + 1} + a_n\frac{P'_n(x; d\mu_0)}{n}, \quad n \geq 1. \quad (5.9)$$

Thus, in the reverse direction, (5.5) leads to (5.9) instead of (5.2).

Evidently, (5.9) is a more general relation than that of (5.2). This suggests the following definition.

Definition 5.5. The pair $\{d\mu_0, d\mu_1\}$ is called a generalized coherent pair if (5.9) holds for all $n \geq 1$, and this definition extends to the linear functionals $\{\mathcal{U}_0, \mathcal{U}_1\}$.

Theorem 5.6. *Let $\mathcal{U}_0, \mathcal{U}_1$ be two linear functionals. Then $\{\mathcal{U}_0, \mathcal{U}_1\}$ is a generalized coherent pair if and only if (5.5) holds.*

Proof. We have already established that (5.5) implies (5.9). Assume now that (5.9) holds. Let $\mathsf{T}_{n+1}(x) := P_{n+1}(x; \mathcal{U}_0) + \widehat{a}_n P_n(x; \mathcal{U}_0)$, where $\widehat{a}_n = (n+1)a_n/n$. For any polynomial p_{n-1} of degree at most $n-1$, it follows directly from the definition that $\langle \mathsf{T}_{n+1}, p_{n-1}\rangle_{\mathcal{U}_0} = 0$ and it follows from (5.9) that $\langle \mathsf{T}'_{n+1}, p'_{n-1}\rangle_{\mathcal{U}_1} = 0$. Consequently, $\langle \mathsf{T}_{n+1}, p_{n-1}\rangle_{\lambda} = 0$. Hence, expanding T_{n+1} in terms of $S_n(x; \lambda)$, we see that

$$\mathsf{T}_{n+1}(x) = S_{n+1}(x; \lambda) + b_n(\lambda) S_n(x; \lambda), \quad n \geq 0,$$

which is precisely (5.5) with n replaced by $n + 1$. $\square$

Two examples of generalized coherent pairs were given in [16,15] when $\mathcal{U}_0$ is a polynomial perturbation of degree 1 of the Laguerre or Jacobi linear functional.

Example 5.7. In these examples, $\{d\mu_0, d\mu_1\}$ is not a coherent pair but a generalized coherent pair. For the first example, $\alpha, \beta > -1$ and $|\xi_0|, |\xi_1| \geq 1$,

$$d\mu_0 = (1 - x)^\alpha (1 + x)^\beta dx, \qquad d\mu_1 = \frac{x - \xi_0}{x - \xi_1}(1 - x)^{\alpha+1}(1 + x)^{\beta+1}dx + M\delta_{\xi_1}.$$

For the second example, $\alpha > -1$ and $\xi \leq 0$,

$$d\mu_0 = x^\alpha e^{-x} dx \qquad d\mu_1 = \frac{x - \xi_0}{x - \xi} x^{\alpha+1} e^{-x} dx + M\delta_\xi.$$

As in the case of coherent pairs, one can ask the question of identifying all generalized coherent pairs. If $\mathcal{U}_0$ is a classical linear functional, then the answer to this question was given in [4]. The complete identification was achieved in [34], which states that either $\mathcal{U}_0$ or $\mathcal{U}_1$ must be a semiclassical linear functional.

Definition 5.8. Let s be a nonnegative integer. A linear functional $\mathcal{U}$ is called semiclassical of class s if there exist polynomials ϕ and ψ such that $s = \max\{\deg\phi - 2, \deg\psi - 1\}$ and $\partial(\phi\mathcal{U}) = \psi\mathcal{U}$.

An in-depth study of orthogonal polynomials with respect to a semiclassical linear functional is given in [83], which contains the following theorem.

Theorem 5.9. *For a semiclassical linear functional $\mathcal{U}$ of class s, the following are equivalent:*

1. *$\{P_n\}_{n \geq 0}$ is a sequence of monic orthogonal polynomials with respect to $\mathcal{U}$;*
2. *There exists a monic polynomial ϕ such that $\langle \phi\mathcal{U}, P'_n Q\rangle = 0$ for all $Q \in \Pi_{n-s-1}$.*
3. *There exists a monic polynomial ϕ of degree r and constants $a_{n,j}$ such that*

$$\phi(x) P'_{n+1}(x) = \sum_{j=n-s}^{n+r} a_{n,j} P_j(x), \quad \text{where } a_{n,n-s} \neq 0.$$

Every semiclassical linear functional of class 0 is classical. The next case, semiclassical of class 1, is used to characterize the generalized coherent pairs. The main result in [34] is the following theorem.

Theorem 5.10. *If $\{\mathcal{U}_0, \mathcal{U}_1\}$ is a generalized coherent pair, then at least one of them has to be semiclassical of class at most* 1.

The proof is based on the observation that if $\{\mathcal{U}_0, \mathcal{U}_1\}$ is a generalized coherent pair, then there are polynomials Q_n of degree n and R_{n+1} of degree at most $n + 1$, such that

$$\partial(Q_n\mathcal{U}_1) = R_{n+1}\mathcal{U}_0, \quad n \geq 1,$$

which is an analogue of (5.7). This relation with $n = 1$ and $n = 2$ is used to deduce the existence of polynomials ϕ of degree at most 4, χ of degree at most 3 and ψ of degree exactly 2, such that

$$\phi\partial\mathcal{U}_1 = \chi\mathcal{U}_1, \qquad \phi\mathcal{U}_0 = \psi\mathcal{U}_1, \qquad \chi\mathcal{U}_0 = \psi\partial\mathcal{U}_1, \tag{5.10}$$

where ϕ, χ and ψ can be given explicitly in terms of R_1, R_2, Q_1 and Q_2. In particular, $\psi = R_1 R_2' - R_2$. This is an analogue of (5.8) for the coherent pair, in which the degrees of ϕ and χ are increased by 1. The polynomial ψ has two zeros. If the two zeros coincide, say at ξ, then it can be shown that $\phi(x) = (x - \xi)\widetilde{\phi}(x)$ and $\mathcal{U}_0$ satisfies $\partial(\widetilde{\phi}\mathcal{U}_0) = \eta\mathcal{U}_0$, where η is a polynomial of degree at most 2. This shows, by Theorem 5.9, that $\mathcal{U}_0$ is semiclassical of class at most 1. In the case of that ψ has two distinct zeros, a more involved analysis shows that ϕ vanishes at one of the zeros, say ξ, so that $\phi(x) = (x - \xi)\widetilde{\phi}(x)$, which can be used to show that $\mathcal{U}_1$ has to be semiclassical of class at most 1. Furthermore, in the latter case, $\mathcal{U}_0$ is determined by $\widetilde{\phi}\mathcal{U}_0 = (x - \xi)\mathcal{U}_1$, where ξ is either one of the two zeros of ψ.

The complete identification of generalized coherent pairs can be worked out by examining all possible $\widetilde{\phi}$. Up to a linear change of variables, if $\deg\widetilde{\phi} = 3$, it has three canonical forms, $\widetilde{\phi}(x) = x^3$, $x^2(x - 1)$, or $x(x - 1)(x - \lambda)$; if $\deg\widetilde{\phi} = 2$, it has two canonical forms, $\widetilde{\phi}(x) = x^2$ or $x(x - 1)$; if $\deg\widetilde{\phi} = 1$, then $\widetilde{\phi}(x) = x$. The arduous work of analyzing all cases was carried out meticulously in [34], where the complete list of generalized coherent pairs can be found in two long tables.

5.4. (M, N) **coherent pairs**

The generalized coherent pair suggests immediately further generalization of coherent pair by extending (5.9).

Definition 5.11. Let M, N and m, n be nonnegative integers. A pair of linear functional $\{\mathcal{U}_0, \mathcal{U}_1\}$ is said to be a (M, N)-coherent pair of order (m, n) if, for $k \geq 0$,

$$\frac{P_{k+m}^{(m)}(x, \mathcal{U}_0)}{(k + 1)_m} + \sum_{i=1}^{M} a_{i,k}\frac{P_{k-i+m}^{(m)}(x, \mathcal{U}_0)}{(k - i + 1)_m} = \frac{P_{k+n}^{(n)}(x, \mathcal{U}_1)}{(k + 1)_n} + \sum_{i=1}^{N} b_{i,k}\frac{P_{k-i+n}^{(n)}(x, \mathcal{U}_1)}{(k - i + 1)_n},$$

where $a_{i,k}$ and $b_{i,k}$ are complex numbers such that $a_{M,k} \neq 0$ if $k \geq M$, $b_{N,k} \neq 0$ if $k \geq N$, and $a_{i,k} = b_{i,k} = 0$ if $i > k$.

In this definition, the coherent pair is the $(1, 0)$-coherent pair of order $(1, 0)$. The generalized coherent pair is $(1, 1)$-coherent pair of order $(1, 0)$. The $(2, 0)$-coherent pair of

order $(1, 0)$ was considered in [63] and the $(M, 0)$-coherent pair of order $(1, 0)$ was called M-coherent pair and studied in [73]. The general setting of (M, N)-coherent pairs of order (m, n) was studied more recently in [31,32,30].

Let $a_{0,k} := 1$ for $0 \leq k \leq N - 1$ and $b_{0,k} := 1$ for $0 \leq k \leq M - 1$. Set

$$
A_N := \begin{bmatrix} a_{0,0} & \cdots & \cdots & a_{M,M} & & \bigcirc \\ & a_{0,1} & \cdots & & \cdots & a_{M,M+1} \\ & & \ddots & \cdots & & \ddots \\ \bigcirc & & & a_{0,N-1} & \cdots & a_{M,M+N-1} \end{bmatrix},
$$

$$
B_M := \begin{bmatrix} b_{0,0} & \cdots & \cdots & b_{N,N} & & \bigcirc \\ & b_{0,1} & \cdots & & \cdots & b_{N,N+1} \\ & & \ddots & \cdots & & \ddots \\ \bigcirc & & & b_{0,M-1} & \cdots & b_{N,M+N-1} \end{bmatrix}, \qquad L_{M+N} := \begin{bmatrix} A_N \\ B_M \end{bmatrix}.
$$

Then A_N is a matrix of size $N \times (M + N)$, B_M is a matrix of size $M \times (M + N)$, and L_{M+N} is a square matrix of size $(M + N) \times (M + N)$.

Theorem 5.12. *Let $\{\mathcal{U}_0, \mathcal{U}_1\}$ be a (M, N)-coherent pair of order (m, n) with $m \geq n$ and assume that L_{M+N} is a non-singular matrix. Then there exist polynomials Q_{M+n+k} of degree $M + n + k$ and R_{N+m+k} of degree at most $N + m + k$, such that*

$$
\partial^{m-n}(Q_{M+n+k}\mathcal{U}_1) = R_{N+m+k}\mathcal{U}_0, \quad k \geq 0. \tag{5.11}
$$

Furthermore, the following classification holds
(1) If $m = n$, then $\mathcal{U}_0$ is semiclassical if and only if $\mathcal{U}_1$ is semiclassical.
(2) If $m > n$, then $\mathcal{U}_0$ and $\mathcal{U}_1$ are both semiclassical.

Eq. (5.11) is an extension of (5.7). This theorem was established in [30] and it extends the results in [31,32,75].

The connection between these extended coherent pairs and the Sobolev orthogonal polynomials is illustrated in the case of (M, N)-coherent pair of order $(m, 0)$, which is called (M, N)-coherent pair of order m. Assume that $\mathcal{U}_0$ and $\mathcal{U}_1$ are positive definite and represented by $d\mu_0$ and $d\mu_1$, respectively. Fix $m \in \mathbb{N}$ and define the Sobolev inner product by

$$
\langle f, g \rangle_\lambda := \int_{\mathbb{R}} f(x)g(x)d\mu_0 + \lambda \int_{\mathbb{R}} f^{(m)}(x)g^{(m)}(x)d\mu_1, \quad \lambda > 0.
$$

Let $\{S_n(\cdot; \lambda)\}$ denote the corresponding sequence of monic orthogonal polynomials.

Theorem 5.13. *Let $\{\mu_0, \mu_1\}$ be a (M, N)-coherent pair of order m. If $n < m$, then $S_n(x; \lambda) = P_n(x; d\mu_1)$ and, for $n \geq 0$,*

$$
\frac{P_{n+m}(x; d\mu_0)}{(n + 1)_m} + \sum_{i=1}^{M} a_{i,n} \frac{P_{n-i+m}(x; d\mu_0)}{(n - i + 1)_m}
$$

$$
= \frac{S_{n+m}(x; \lambda)}{(n + 1)_m} + \sum_{j=n+1}^{\max\{M,N\}} c_{j,n}(\lambda) \frac{S_{n-j+m}(x; \lambda)}{(n - j + 1)_m},
$$

where $c_{j,n}(\lambda)$ are constants that can be determined recursively.

This theorem was also established in [30], where an algorithm is given for computing $c_{j,n}(\lambda)$ and the Fourier coefficients of the orthogonal expansion in $S_n(\cdot; \lambda)$.

As in the case of coherent or generalized coherent pairs, one can consider the problem of identifying all coherent pairs. The problem, however, is open in all cases beyond the two cases that we have discussed. At the time of this writing, the (M, N)-coherent pairs of order (m, n) are still under study.

6. Classical orthogonal polynomials as Sobolev orthogonal polynomials

The classical orthogonal polynomials are Sobolev orthogonal polynomials themselves, since derivatives of a classical orthogonal polynomial are classical orthogonal polynomials of the same type. Indeed, for the Hermite polynomials H_n, $H_n'(x) = 2nH_{n-1}(x)$, so that $\{H_n\}_{n\geq 0}$ is also the sequence of orthogonal polynomials with respect to the Sobolev inner product

$$\langle f, g\rangle_{\mathcal{H}} := \sum_{k=0}^{m} \lambda_k \int_{\mathbb{R}} f^{(k)}(x)g^{(k)}(x)e^{-x^2}dx, \quad m = 1, 2, \ldots, \tag{6.1}$$

where $\lambda_0 > 0$ and $\lambda_k \geq 0$ for $k = 1, \ldots, m$, which we assume for the two cases below as well. For the Laguerre polynomials $L_n^{(\alpha)}$, $\frac{d}{dx}L_n^{(\alpha)}(x) = -L_{n-1}^{(\alpha+1)}(x)$, so that $\{L_n^{(\alpha)}\}_{n\geq 0}$ is also the sequence of orthogonal polynomials with respect to the Sobolev inner product

$$\langle f, g\rangle_{\mathcal{L}^\alpha} := \sum_{k=0}^{m} \lambda_k b^{(\alpha+k)} \int_0^\infty f^{(k)}(x)g^{(k)}(x)x^{\alpha+k}e^{-x}dx, \quad m = 1, 2, \ldots, \tag{6.2}$$

where $b^{(\alpha)} := 1/\Gamma(\alpha + 1)$ and $\alpha > -1$. For the Jacobi polynomials $P_n^{(\alpha,\beta)}$, it is known that $\frac{d}{dx}P_n^{(\alpha,\beta)}(x) = \frac{n+\alpha+\beta+1}{2}P_{n-1}^{(\alpha+1,\beta+1)}(x)$, so that $\{P_n^{(\alpha,\beta)}\}_{n\geq 0}$ is also the sequence of the orthogonal polynomials with respect to the Sobolev inner product

$$\langle f, g\rangle_{\mathcal{J}^{\alpha,\beta}} := \sum_{k=0}^{m} \lambda_k b^{(\alpha+k,\beta+k)} \int_{-1}^{1} f^{(k)}(x)g^{(k)}(x)(1-x)^{\alpha+k}(1+x)^{\beta+k}dx, \tag{6.3}$$

where $m = 1, 2, \ldots$ and $b^{(\alpha,\beta)} := \Gamma(\alpha + \beta + 2)/(2^{\alpha+\beta+1}\Gamma(\alpha + 1)\Gamma(\beta + 1))$, and $\alpha, \beta > -1$.

For arbitrary $\alpha \in \mathbb{R}$, the Laguerre polynomials can be defined by the explicit formula [101, (5.1.6)]

$$L_n^{(\alpha)}(x) = \sum_{\nu=0}^{n} \frac{(\alpha + \nu + 1)_{n-\nu}}{(n-\nu)!} \frac{(-x)^\nu}{\nu!}, \quad n \geq 0,$$

which turns out to be orthogonal with respect to a Sobolev inner product. For $k \in \mathbb{N}$, define a matrix $M(k)$ by

$$M(k) = \left[m_{i,j}(k)\right]_{i,j=0}^{k} := Q(k)Q(k)^T, \quad Q(k) := \left[(-1)^{j-i}\binom{k-i}{j-i}\right]_{i,j=0}^{k},$$

where we assume that $\binom{a}{b} = 0$ if $b < 0$. Then $M(k)$ is positive definite.

Theorem 6.1. *For $\alpha \in \mathbb{R}$, let $k := \max\{0, \lfloor \alpha \rfloor\}$. Then the sequence of Laguerre polynomials $\{L_n^{\alpha}\}_{n \geq 0}$ is orthogonal with respect to the inner product*

$$\langle f, g \rangle_{\mathcal{L}^{\alpha}} := \int_0^{\infty} \left(f(x), f'(x), \ldots, f^{(k)}(x) \right) M(k)$$
$$\times \left(g(x), g'(x), \ldots, g^{(k)}(x) \right)^T x^{\alpha+k} e^{-x} dx.$$

Moreover, if $-\alpha \in \mathbb{N}$, then $k = -\alpha$ and one can write, by integration by parts,

$$\langle f, g \rangle_{\mathcal{L}^{-k}} = \frac{1}{2} \sum_{i=0}^{k-1} \sum_{j=0}^{i} m_{i,j}(k) \left[f^{(i)}(0) g^{(j)}(0) + f^{(j)}(0) g^{(i)}(0) \right]$$
$$+ \int_0^{\infty} f^{(k)}(x) g^{(k)}(x) e^{-x} dx.$$

This theorem was proved in [95]. The case $-\alpha \in \mathbb{N}$ was proved in [64]. In the case of $-\alpha \in \mathbb{N}$, the result can be deduced directly with the help of the relation

$$L_n^{(-k)}(x) = (-x)^k \frac{(n-k)!}{n!} L_{n-k}^{(k)}(x), \quad n \geq k, \tag{6.4}$$

which shows, in particular, that $L_n^{(-k)}$ and its up to $(k-1)$th derivatives vanish at $x = 0$, so that the orthogonality follows immediately from $\frac{d}{dx} L_n^{(\alpha)}(x) = -L_{n-1}^{(\alpha+1)}(x)$.

In the Jacobi case, it is known that if $-\alpha, -\beta, -\alpha - \beta \in \mathbb{R} \setminus \mathbb{N}$, then the Jacobi polynomials are orthogonal with respect to some Sobolev inner product of the form

$$\langle f, g \rangle = \int_{\mathbb{R}} f(x) g(x) d\mu_0(x) + \int_{\mathbb{R}} f'(x) g'(x) d\mu_1(x),$$

where μ_0 and μ_1 are real, possibly signed, Borel measure on $\mathbb{R}$. In the case of $\alpha = -k, k \in \mathbb{N}$, and $-\beta - k \in \mathbb{R} \setminus \mathbb{N}$, more can be said since

$$\binom{n}{k} P_n^{(-k,\beta)}(x) = \binom{n+\beta}{k} \left(\frac{x-1}{2} \right)^k P_{n-k}^{(k,\beta)}(x), \tag{6.5}$$

and an analogous expression for $P_n^{(\alpha,-k)}$ follows from $P_n^{(\alpha,\beta)}(x) = (-1)^n P_n^{(\beta,\alpha)}(-x)$. It follows that the $P_n^{(-k,\beta)}$ and its up to $(k-1)$th derivatives vanish at $x = 1$. Furthermore, $\frac{d^k}{dx^k} P_n^{(-k,\beta)}(x) = c P_{n-k}^{(0,\beta+k)}(x)$. These relations can be used to derive a Sobolev orthogonality of the Jacobi polynomials. Let $\Lambda(k) = \text{diag}\{\lambda_1, \ldots, \lambda_k\}$ with $\lambda_j > 0$. Define

$$M(k) = Q(k)^{-1} \Lambda(k) (Q(k)^{-1})^T, \quad Q(k) = \left[\left(\partial^j P_i^{(-k,\beta)} \right)(1) \right]_{i,j=0}^{k-1}.$$

Theorem 6.2. *For $k \in \mathbb{N}$ and $\beta \in \mathbb{R}$ such that $-(k+\beta) \notin \mathbb{N}$, the sequence of Jacobi polynomials $\{P_n^{(-k,\beta)}\}_{n \geq 0}$ is orthogonal with respect to the inner product*

$$\langle f, g \rangle_{\mathcal{J}^{-k,\beta}} := \int_{-1}^{1} f^{(k)}(x) g^{(k)}(x)(1+x)^{k+\beta} dx$$
$$+ \left(f(1), f'(1), \ldots, f^{(k-1)}(1) \right) M(k) \left(g(1), g'(1), \ldots, g^{(k)}(1) \right)^{T}.$$

An analogue result can be stated for $\alpha \in \mathbb{R}$ and $-(\alpha + k) \notin \mathbb{N}$, where the point evaluations need to be at -1. This theorem was proved in [8], which contains an analogue result for the Laguerre polynomials $L_n^{(-k)}$ that is more general than the corresponding result in Theorem 6.1. These results extend several special cases appeared early in the literature (see, for example, [65]).

Similar results also hold for the Jacobi polynomials with $\alpha = -k, \beta = -l$ with $k, l \in \mathbb{N}$, where the orthogonality is defined with respect to the bilinear form

$$\langle f, g \rangle = \int_{-1}^{1} f^{(k+l)}(x) g^{(k+l)}(x)(1-x)^l (1+x)^k dx + \langle f, g \rangle_D,$$

where $\langle f, g \rangle_D$ is defined via point evaluations of f and g and their derivatives up to $(k-1)$th order at 1 and up to $(l-1)$th order at -1 [2,10]. In this case, the Jacobi polynomial $P_n^{(-k,-l)}$ vanishes identically for $\max\{k, l\} \le n < k + l$ and has reduced degree if $(k+l)/2 \le n < \max\{k, l\}$, so that it is necessary to define the Jacobi polynomials with such indexes. There are several ways to redefine these polynomials. Let $\widehat{P}_n^{(\alpha,\beta)}$ denote the usual monic Jacobi polynomial of degree n. In [2], the monic Jacobi polynomials $\widehat{P}_n^{(k,-l)}$ are defined by

$$\widehat{P}_n^{(k,-l)}(x) = \frac{1}{2} \left[\lim_{\alpha \to -k} P_m^{(\alpha,-l)}(x) + \lim_{\beta \to -l} P_m^{(-k,\beta)}(x) \right],$$

where $m = k + l - n - 1$ if $(k+l)/2 \le n < \max\{k, l\}$ and $m = n$ otherwise.

It is worth mentioning that the Jacobi polynomials with negative indexes have been used extensively in the spectral theory for solving differential equations. See, for example, [49,68,69,100] and the references therein. In the spectral theory, orthogonal expansions and approximation by polynomials in Sobolev spaces are used, so that Sobolev orthogonal polynomials are needed, although they often appear implicitly.

7. Sobolev type orthogonal polynomials

As stated in the introduction, an inner product is called a Sobolev type inner product if the derivatives appear only on function evaluations on a finite discrete set. More precisely, such an inner product takes the form

$$\langle f, g \rangle_S := \int_{\mathbb{R}} f(x) g(x) d\mu_0 + \sum_{k=1}^{m} \int_{\mathbb{R}} f^{(k)}(x) g^{(k)}(x) d\mu_k, \qquad (7.1)$$

where $d\mu_0$ is a positive Boreal measure supported on an infinite subset of the real line and $d\mu_k, k = 1, 2, \ldots, m$, are positive Borel measures supported on finite subsets of the real line. Let δ_c denote the delta measure supported at the point $c \in \mathbb{R}$, that is, $\delta_c f(x) = f(c)$.

In most cases considered below, $d\mu_k = A_k\delta_c$ or $d\mu_k = A_k\delta_a + B_k\delta_b$, where A_k and B_k are nonnegative numbers.

Orthogonal polynomials for such an inner product are called either Sobolev type orthogonal polynomials or discrete Sobolev orthogonal polynomials. The first study was carried out for the classical weight functions. The Laguerre case was studied in [57] with $d\mu_0 = x^\alpha e^{-x}dx, \alpha > -1$, and $d\mu_k = M_k\delta_0, k = 1, 2, \ldots, m$; the nth Sobolev orthogonal polynomial, S_n, is given by

$$S_n(x) = \sum_{k=0}^{\min\{n,m+1\}} (-1)^k A_k L_{n-k}^{\alpha+k}(x),$$

in which A_k are constants determined by a linear system of equations. The Gegenbauer case was studied in [13,14] with $d\mu_0 = (1 - x^2)^{\lambda-1/2}dx + A(\delta_{-1} + \delta_1), \lambda > -1/2$, and $m = 1, d\mu_1 = B(\delta_{-1} + \delta_1)$; the nth Sobolev orthogonal polynomial is given by

$$S_n(x) = \sum_{k=0}^{2} a_{k,n}x^k C_{n-k}^{\lambda+k}(x)$$

where $a_{0,n}, a_{1,n}, a_{2,n}$ are appropriate constants. In both cases, the Sobolev orthogonal polynomials satisfy higher (than three) order recurrence relations that expands $q(x)S_n(x)$ as a sum of S_m. For the Laguerre case, $q(x) = x^{m+1}$ and the order is $2m + 3$; for the Gegenbauer case, either $q(x) = (1 - x^2)^2$ and the order is 9 or $q(x) = x^3 - 3x$ and the order is 7. Furthermore, in both cases, the polynomial S_n satisfies a second order linear differential equation with polynomial coefficients, whose degree does not depend on n.

When $M_k = 0, k = 1, 2, \ldots, m-1$, and $d\mu_m = M_m\delta_c$, the inner product (7.1) becomes

$$\langle f, g \rangle_m := \int_{\mathbb{R}} f(x)g(x)d\mu_0 + M_m f^{(m)}(c)g^{(m)}(c), \tag{7.2}$$

where $c \in \mathbb{R}$ and $M_m \geq 0$. This case was studied in [80]. Let $\{P_n\}_{n\geq 0}$ and $\{S_n\}_{n\geq 0}$ denote the sequences of monic orthogonal polynomials with respect to $d\mu_0$ and $\langle \cdot, \cdot \rangle_m$, respectively. For $i, j \in \mathbb{N}_0$, define

$$K_{n-1}^{(i,j)}(x, y) := \sum_{l=0}^{n-1} \frac{P_l^{(i)}(x)P_l^{(j)}(y)}{\|P_l\|_{d\mu_0}^2}.$$

Notice that $K_{n-1}^{(0,0)}$ is the reproducing kernel of the $(n - 1)$th partial sum of orthogonal expansion with respect to $d\mu_0$. It was shown in [80] that

$$S_n(x) = P_n(x) - \frac{M_m P_n^{(m)}(c)}{1 + M_m K_{n-1}^{(m,m)}(c, c)} K_{n-1}^{(0,m)}(x, c), \tag{7.3}$$

which extends the expression for $m = 0$ in [62]. From this relation, one deduces immediately that

$$S_{n+1}(x) + a_n S_n(x) = P_{n+1}(x) + b_n P_n(x), \quad n \geq 0,$$

where a_n and b_n are constants that can be easily determined. This shows a structure similar to (5.5) that one derives for the Sobolev orthogonal polynomials in the case of coherent pair. The Sobolev polynomials S_n also satisfy a higher order recurrence relation

$$(x - c)^{m+1} S_n(x) = \sum_{j=n-m-1}^{n+m+1} c_{n,j} S_j(x), \tag{7.4}$$

where $c_{n,n+m+1} = 1$ and $c_{n,n-m-1} \neq 0$.

Orthogonality of a sequence of polynomials is determined by the three term recurrence relations that it satisfies, the precise statement is known as the Favard theorem. One may ask if there is a similar theorem for polynomials satisfying higher order recurrence relations. There are two types of results in this direction, both related to Sobolev orthogonal polynomials.

The first one gives a characterization of an inner product $\langle \cdot, \cdot \rangle$ for which orthogonal polynomials satisfy the recurrence relation of the form (7.4), which holds if the operator of multiplication by $M_{m,c} := (\cdot - c)^{m+1}$ is symmetric, i.e., $\langle M_{m,c} p, q \rangle = \langle p, M_{m,c} q \rangle$. It was proved in [39] that if $\langle \cdot, \cdot \rangle$ is an inner product such that $M_{m,c}$ is symmetric and it commutes with the operator $M_{0,c}$, i.e., $\langle M_{m,c} p, M_{0,c} q \rangle = \langle M_{0,c} p, M_{m,c} q \rangle$, then there exists a nontrivial positive Borel measure $d\mu_0$ and a real, positive semi-definite matrix A of size $m + 1$, such that the inner product is of the form

$$\langle p, q \rangle = \int_{\mathbb{R}} p(x)q(x)d\mu_0$$
$$+ \left(p(c), p'(c), \ldots, p^{(m)}(c) \right) A \left(q(c), q'(c), \ldots, q^{(m)}(c) \right)^T. \tag{7.5}$$

Necessary and sufficient conditions for A being diagonal were also given in [39]. Furthermore, a connection between such Sobolev orthogonal polynomials and matrix orthogonal polynomials was established in [41], by representing the higher order recurrence relation as a three term recurrence relation with matrix coefficients for a family of matrix orthogonal polynomials defined in terms of the Sobolev orthogonal polynomials.

The second type of Favard type theorem was given in [42], where it was proved that the operator of multiplication by a polynomial h is symmetric with respect to the inner product (7.1) if and only if $d\mu_k, k = 1, 2, \ldots, m$, are discrete measures whose supports are related to the zeros of h and their derivatives. Consequently, higher order recurrence relations for Sobolev inner products appear only in Sobolev inner product of the second type.

For the inner product (7.5), a sequence of Sobolev orthogonal polynomials can be constructed using an extension of the method used to obtain (7.1). A more useful approach is to use the monic orthogonal polynomials, $\widehat{P}_n$, with respect to the measure $d\mu_0^* = (x - c)^p d\mu_0$, where $p = 2\lfloor m/2 \rfloor + 2$, which leads to [42]

$$S_n(x) = \sum_{k=0}^{p} d_{n,k} \widehat{P}_{n-k}(x), \quad n \geq p, \tag{7.6}$$

where $d_{n,0} = 1$ and $d_{n,p} \neq 0$. The above relation means that the sequence $\{S_n\}_{n \geq 0}$ is quasi-orthogonal with respect to the positive Borel measure $d\mu_0^*$, a fact that plays a central

role in the analysis of zeros and asymptotics of these polynomials. If the point c is located outside the support of the measure $d\mu_0$, it is enough to consider $d\mu_0^* = (x - c)^{m+1} d\mu_0$, in which case, (7.6) is satisfied with $m + 1$ instead of p and the formula has the minimal length. If c belongs to the support of the measure $d\mu_0$ and m is an even integer, then $(x - c)^{m+1} d\mu_0$ becomes a signed measure, which does not warrant the existence of orthogonal polynomials. This is the reason behind the definition of p in (7.6). Let H be the banded matrix that defines the higher order recurrence relation for $\{S_n\}_{n \geq 0}$. Then H can be derived from the Jacobi matrix $\widehat{J}$ associated with the sequence $\{\widehat{P}_n\}_{n \geq 0}$ of monic orthogonal polynomials. Indeed, consider the decomposition $(\widehat{J} - cI)^p = UL$, where U is an upper triangular matrix and L is a lower triangular matrix with 1 as its diagonal entries, then $H = LU$ [36]. This gives a direct connection between Sobolev orthogonal polynomials of discrete type and the iteration of the canonical Geronimus transformation of the measure $d\mu^* = (\cdot - c) d\mu$.

8. Differential equations

Classical orthogonal polynomials are solutions of a second order linear differential equation of the form

$$\alpha_2(x) y'' + \alpha_1(x) y' = -\lambda_n y, \quad n = 0, 1, \ldots, \tag{8.1}$$

where α_2 and α_1 are real-valued functions and λ_n are real numbers, called eigenvalues. The equation is called admissible if $\lambda_n \neq \lambda_m$ whenever $n \neq m$. For Eq. (8.1) to have a system of polynomial solutions, it is necessary that α_2 is a polynomial of degree at most 2 and α_1 is a polynomial of degree at most 1. For $n = 0, 1, \ldots$, the Hermite polynomials H_n satisfy the equation

$$D_{\mathcal{H}} y := y'' - 2xy' = -2ny. \tag{8.2}$$

For $\alpha > -1$ and $n = 0, 1, \ldots$, the Laguerre polynomials $L_n^{(\alpha)}$ satisfy the equation

$$D_{\mathcal{L}}^\alpha y := xy'' + (\alpha + 1 - x) y' = -ny. \tag{8.3}$$

For $\alpha, \beta > -1$ and $n = 0, 1, \ldots$, the Jacobi polynomials $P_n^{(\alpha,\beta)}$ satisfy the equation

$$D_{\mathcal{J}}^{\alpha,\beta} y := (1 - x^2) y'' - (\alpha - \beta + (\alpha + \beta + 2)x) y' = -n(n + \alpha + \beta + 1) y. \tag{8.4}$$

The characterization of Bochner [17] shows that these are essentially the only systems of orthogonal polynomials with respect to a positive definite inner product $\langle f, g \rangle_{d\mu} = \int_{\mathbb{R}} f(x) g(x) d\mu$ that satisfy (8.1). For the quasi-definite linear functional, the condition for the Laguerre family can be relaxed to $-\alpha \in \mathbb{R} \setminus \mathbb{N}$, and the condition for the Jacobi family can be relaxed to $-\alpha, -\beta, -(\alpha + \beta + 1) \in \mathbb{R} \setminus \mathbb{N}$, and, up to a complex change of variables, the only other system of orthogonal polynomials that satisfies (8.1) is the system of Bessel polynomials.

Eq. (8.1) have solutions that are Sobolev orthogonal polynomials, since classical orthogonal polynomials are Sobolev orthogonal polynomials themselves. One may ask the question if there are other system of Sobolev orthogonal polynomials that are solutions

of (8.1). In [65], the system of polynomials that are solutions of admissible (8.1) and are orthogonal with respect to the bilinear form

$$\langle f, g \rangle = \int_{\mathbb{R}} f(x)g(x)d\mu_0(x) + \int_{\mathbb{R}} f'(x)g'(x)d\mu_1(x)$$

is characterized when $d\mu_0$ and $d\mu_1$ are real, possibly signed, Borel measures on the real line. The classical orthogonal polynomials and those obtained above through limiting process are the only systems of polynomials in the positive definite case. In the Laguerre case, the limit is

$$\lim_{\alpha \to -1} \frac{1}{\Gamma(\alpha + 1)} \int_0^\infty f(x)x^\alpha e^{-x}dx = f(0),$$

which holds if f is bounded on $(0, \infty)$ and continuous at $x = 0$, and it follows that the system of polynomials $P_0(x) = 1$ and $P_n(x) := L_n^{(-1)}(x)$ for $n \geq 1$ is orthogonal with respect to the Sobolev inner product

$$\langle f, g \rangle_{\mathcal{L}^{-1}} = \lambda_0 f(0)g(0) + \sum_{k=1}^m \lambda_k b^{(k-1)} \int_0^\infty f^{(k)}(x)g^{(k)}(x)x^{k-1}e^{-x}dx,$$

where $\lambda_0, \lambda_1 > 0$ and $\lambda_k \geq 0$ for $2 \leq k \leq m, b^{(k-1)}$ is as in formula (6.2), and these polynomials are solutions of the differential equation $D_{\mathcal{L}}^{-1}y = -ny$. In the Jacobi case, the limits are

$$\lim_{\alpha \to -1} (\alpha + 1) \int_{-1}^1 f(x)(1 - x)^\alpha dx = f(1),$$

$$\lim_{\beta \to -1} (\beta + 1) \int_{-1}^1 f(x)(1 + x)^\beta dx = f(-1),$$

which hold if f is bounded on $(-1, 1)$ and continuous at $x = 1$ or $x = -1$, respectively, and it follows that, for $\beta > -1$, the system of polynomials $P_0(x) = 1$ and $P_n(x) := P_n^{(-1,\beta)}(x)$ for $n \geq 1$ is orthogonal with respect to the Sobolev inner product

$$\langle f, g \rangle_{\mathcal{J}^{-1,\beta}} = \lambda_0 f(1)g(1)$$
$$+ \sum_{k=1}^m \lambda_k b^{(k-1,\beta)} \int_{-1}^1 f^{(k)}(x)g^{(k)}(x)(1 - x)^{k-1}(1 + x)^{\beta+k}dx,$$

where $\lambda_0, \lambda_1 > 0$ and $\lambda_k \geq 0$ for $2 \leq k \leq m, b^{(k-1,\beta)}$ is as in formula (6.3), and these polynomials are solutions of the differential equation $D_{\mathcal{J}}^{-1,\beta}y = -n(n + \beta)y$. A similar result holds for $\alpha > -1$ and $\beta = -1$. The characterization in [65] was carried out for the quasi-definite case, which shows that, up to a complex linear change of variables, the only systems are those listed above but with parameters being real numbers, except negative integers, and Bessel polynomials.

Essentially, solutions of the second order differential equation (8.1) do not lead to new families of Sobolev orthogonal polynomials; see [8,65] for further results.

In [58], R. Koekoek initiated a search for differential operators whose solutions are the Sobolev–Laguerre polynomials with respect to the inner product

$$\langle f, g \rangle = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty f(x)g(x)x^a e^{-x}dx + Mf(0)g(0) + Nf'(0)g'(0),$$

where $\alpha > -1$, $M \geq 0$ and $N \geq 0$. These Sobolev orthogonal polynomials were found in [60] and they satisfy differential equations of the form

$$M \sum_{i=0}^\infty a_i(x)y^{(i)}(x) + N \sum_{i=0}^\infty b_i(x)y^{(i)}(x)$$

$$+ MN \sum_{i=0}^\infty c_i(x)y^{(i)}(x) + xy''(x) + (\alpha+1-x)y'(x) = -ny,$$

where $a_i(x)$, $b_i(x)$ and $c_i(x)$ are polynomials, independent of n, of degree at most i. In the case of $M = 0$ and $N > 0$, the differential equation is of order $2\alpha + 8$ if α is a nonnegative integer and of infinite order otherwise. Furthermore, if $M > 0$ and $N > 0$, then the differential equation is of order $4\alpha + 10$ if α is a nonnegative integer and of infinite order otherwise. For $\alpha = 0, 1, 2$, this was established in [58] and the general case was proved in [59].

This result has been extended more recently to the Sobolev orthogonal polynomials with respect to the bilinear form

$$\langle f, g \rangle = \int_0^\infty f(x)g(x)x^{\alpha-m}e^{-x}dx$$

$$+ \left(f(0), f'(0), \dots, f^{(m-1)}(0) \right) M \left(g(0), g'(0), \dots, g^{(m-1)}(0) \right)^T,$$

where $m = 2, 3, \dots$, and M is an $m \times m$ matrix. For $m = 2$, the differential operator was found in [53] and for $\alpha \in \mathbb{N}$ and $\alpha \geq m$, the differential operator was constructed in [40].

9. Zeros

It is well known that the zeros of orthogonal polynomials with respect to a probability measure supported on the real line are real, simple, interlace and are located in the interior of the convex hull of the support of the measure. In the Sobolev setting, some of the above properties are lost. We will specify the behavior of zeros for two types of Sobolev orthogonal polynomials.

9.1. Sobolev type inner products

Here we consider the Sobolev inner product defined in (7.5), which we state again as

$$\langle p, q \rangle = \int_I p(x)q(x)d\mu_0$$

$$+ \left(p(c), p'(c), \dots, p^{(m)}(c) \right) A \left(q(c), q'(c), \dots, q^{(m)}(c) \right)^T, \qquad (9.1)$$

where I is an interval in $\mathbb{R}$, and we denote by S_n a Sobolev orthogonal polynomial of degree n with respect to this inner product.

We start with zeros of Sobolev orthogonal polynomials for the inner product

$$\langle f, g \rangle_S = \int_0^a f(x)g(x)d\mu_0(x) + M_1 f^{(r)}(0)g^{(r)}(0) + M_2 f^{(s)}(0)g^{(s)}(0), \quad r < s,$$

studied in [28], where it was shown that the polynomial S_n of degree n has exactly $n - 2$ real and simple zeros in $(0, a)$, and if $s = r + 1$, then S_n has a pair of conjugate complex zeros $\alpha \pm i\beta$ with $\alpha < 0$ and $\beta \neq 0$, whereas if $s > r + 1$, then there is a real number G such that if $\min\{M_1, M_2\} > G$, then S_n has either a pair of conjugate complex zeros as above or two real zeros in $(-\infty, 0)$.

These results illustrate that the behavior of the zeros of Sobolev orthogonal polynomials for the inner product (9.1) is sensitive to small changes in the parameters of the inner product.

Next we describe the results for the simplest case of $m = 1$ in (9.1). If $A = \mathrm{diag}\{A_0, A_1\}$ and $m = 1$, the polynomial S_n is quasi-orthogonal of order 2 with respect to the measure $(x - c)^2 d\mu_0$; that is, $\int_I S_n(x)p(x)(x - c)^2 d\mu_0 = 0$ for all polynomials p of degree at most $n - 3$. The zeros of S_n were analyzed in [5], where it was proved that the zeros of S_n are real, simple, and at least $n - 1$ of them belong to the interval I of the support of $d\mu_0$, when c is an end point of the interval I. More precisely, let the zeros be denoted by $z_{k,n}, k = 1, 2, \ldots, n$, and they are arranged in increasing order with $z_{n,n}$ being the largest one. If $c = \sup I$ and neither $S_n(c) > 0$ nor $S_n'(c) > 0$, then the largest zero satisfies $c \leq z_{n,n} < c + \frac{c - z_{1,n}}{n-1}$ and $|z_{n,n} - c| < |z_{n-1,n} - c|$. Moreover, if $A_0 \neq 0$, then $z_{n,n} - c < \frac{1}{2}(A_1/A_0)^{1/2}$. Making a change of variable $x \mapsto -x$ in the inner product, the same analysis applies to the case of $c = \inf I$.

The case when c is outside of the convex hull of the support of $d\mu_0$ was analyzed in [76] under the assumption that $A_0 = 0$. In this case, S_n again has real, simple zeros and at least $n - 1$ of them belong to I. If I is a bounded interval, then for n large enough and $c > \sup I$, S_n has a zero at the right hand side of c. This zero converges to c when n tends to infinity, that is, c becomes an attractor of this exceptional zero. Furthermore, the zeros of $P_{n-1}(\cdot; d\mu_0)$ interlace with the zeros of S_n. Finally, it was proved that every zero of S_n is an increasing and bounded function of N.

When the matrix A in (9.1) is a non-diagonal matrix, the case $m = 1$ was studied in [6]. Assuming that A is positive definite, it was shown that if I is a bounded interval and $c > \sup I$, then there exists a positive integer n_0 such that, for $n \geq n_0$, the zeros of S_n are real, simple, all except the largest one are located in $(\inf I, c)$, whereas the largest zero is greater than c. Furthermore, if the non-diagonal entry $A_{0,1}$ is positive, then more can be said on the distance from the largest zero to c,

(1) If $A_{0,0}A_{1,1} \geq 2A_{0,1}^2$, then $z_{n,n} - c < \frac{A_{1,1}}{2(A_{0,0}A_{1,1} - A_{0,1}^2)^{1/2}}$.

(2) If $A_{0,1}^2 \geq A_{0,0}A_{1,1} \geq 2A_{0,1}^2$, then $z_{n,n} - c < A_{0,1}/A_{0,0}$.

If $m > 1$ and A is a diagonal matrix, the zeros of S_n were studied in [3]. In this case, S_n is quasi-orthogonal of order $m + 1$ with respect to the measure $(x - c)^{m+1} d\mu_0$ as in (7.6). If c does not belong to the interior of the interval I that supports $d\mu_0$, S_n has at least $n - m - 1$ zeros with odd multiplicity in the interior of I, whenever $n \geq m + 1$. More generally, let $B(\mu_0)$ denote the support of the measure $d\mu_0$ and let Δ denote the convex

hull of $B(\mu_0)$. If $\bar{n}$ denote the number of terms in the discrete part of (9.1) whose order of derivative is less than n, then S_n has at least $n - \bar{n}$ changes of sign in the interior of Δ. Furthermore, if C_α denote the open connected components of $\text{Int}\Delta \setminus B(\mu_0)$, then, for $n > m + 1$, the number of zeros of the polynomial S_n located in each component C_α is less than or equal to either $m + 1$ or $m + 2$, when m is even or odd, respectively. Further refined results on the locations of zeros in C_α can be found in [3].

9.2. Continuous Sobolev inner products

Zeros of Sobolev orthogonal polynomials with respect to the inner product

$$\langle f, g \rangle_S = \int_{\mathbb{R}} f(t)g(t)d\mu_0 + \int_{\mathbb{R}} f'(t)g'(t)d\mu_1 \tag{9.2}$$

were studied in the very beginning of Sobolev orthogonal polynomials. In [9], Althammer proved that the zeros of S_n are real, simple and are located in the interval $[-1, 1]$ when $d\mu_0 = dx$ and $d\mu_1 = \lambda dx$, both supported on the interval $[-1, 1]$. Similar results were established by Brenner [20] for $d\mu_0 = e^{-x}dx$ and $d\mu_1 = \lambda e^{-x}dx$, both supposed on $[0, \infty)$. As already mentioned in Section 2, Althammer gave an example that shows the zeros of a Sobolev orthogonal polynomials of degree 2 can have a zero outside the support of the measures. An interesting example in this regard appears in [90], for which $d\mu_0 = dx$ on $[-1, 3]$, $d\mu_1(x) = \lambda$ on $[-1, 1]$ and $d\mu_1(x) = 1$ on $[1, 3]$, where $\lambda > 0$. For λ sufficiently large, it was shown that S_{2n} has exactly two real zeros, one in $(1, 3)$ and one in $(-3, -1)$, and S_{2n+1} has exactly one real zero, located in $(1, 3)$. The example was generalized to the situation that $d\mu_0$ has at least one point of increasing in $(1, a]$, where $a > 1$, $d\mu_1 = \lambda d\mu_0$ on $[-1, 1]$ and $d\mu_1 = d\mu_0$ on $[1, a]$, with $\mu_2'(x) \geq c > 0$ on $(-1, 1)$.

Zeros of Sobolev orthogonal polynomials are fairly well understood when $(d\mu_0, d\mu_1)$ is a coherent pair. In this paragraph, we follow the notation in Section 5.1. For the inner product $\langle \cdot, \cdot \rangle_\lambda$ in (5.1), we denote the Sobolev orthogonal polynomials by $S_n(\cdot; \lambda)$ and denote the ordinary orthogonal polynomial with respect to $d\mu_i$ by $P_n(\cdot; d\mu_i)$. Let I_0 denote the support of the measure $d\mu_0$. It was proved in [93] that $S_n(\cdot; \lambda)$ has n real, simple zeros and at most one of them is outside I_0. Furthermore, if $(z_{k,n}^\lambda)_{k=1}^n$ and $(x_{k,n}(d\mu_j))_{k=1}^n$, denote the zeros of $S_n(\cdot; \lambda)$ and $P_n(\cdot; d\mu_j)$, respectively, then

(1) $z_{1,n}^\lambda < x_{1,n}(d\mu_0) < z_{2,n}^\lambda < \cdots < z_{n,n}^\lambda < x_{n,n}(d\mu_0)$,
(2) $z_{1,n}^\lambda < x_{1,n-1}(d\mu_j) < z_{2,n}^\lambda < \cdots < x_{n-1,n-1}(d\mu_j) < z_{n,n}^\lambda$, $j = 0, 1$.

Interlacing property between the zeros of two consecutive Sobolev orthogonal polynomials, that is,

$$z_{1,n}^\lambda < z_{1,n-1}^\lambda < z_{2,n}^\lambda < \cdots < z_{n-1,n-1}^\lambda < z_{n,n}^\lambda,$$

holds when $d\mu_0$ and $d\mu_1$ are both Laguerre weight or both Jacobi weights.

If $\{d\mu_0, d\mu_1\}$ is a generalized coherent pair (see Section 5), however, few results on zeros of Sobolev orthogonal polynomials are known. The case of $(2, 0)$ coherent pairs of order $(1, 0)$ was analyzed in [29], where it was shown that if λ is large enough, then the zeros of $S_n(\cdot; \lambda)$ are real, simple and interlace with the zeros of $P_n(\cdot; d\mu_j)$, $j = 0, 1$, when $I_0 = I_1$; furthermore, at most two of the zeros are outside I_0. In [94] an illustrative example

of $(0, 2)$ coherent pair of order $(1, 0)$ associated with Freud weights was studied, in which the zeros of $S_n(\cdot, \lambda)$ are shown to be real, simple and enjoy a separation property.

For the inner product (9.2), potential theoretic method was used in [45] to study asymptotic distribution of zeros and critical points Sobolev orthogonal polynomials. Under the assumption that the support I_j of the measure $d\mu_j$ is compact and regular for the Dirichlet problem in $\overline{\mathbb{C}} \setminus I_j$ for $j = 0, 1$ and further regularity assumption, it was proved that the critical points, or zeros of the derivative of S_n, have a canonical asymptotic distribution supported on the real line; that is, their counting measure converges weakly to the equilibrium measure of the union $\Sigma = I_0 \cup I_1$. For the zeros of S_n, it was shown that the weak* limit of a subsequence of their counting measure is supported on a subset of $\Sigma \cup \bar{V}$, where $V = \cup_{r>0} V_r$ and V_r denotes the union of those components of $\{z \in \mathbb{C} : g_{\bar{\mathbb{C}} \setminus \Sigma}(z; \infty) < r\}$ having empty intersection with I_0, in which $g_A(z; \infty)$ denotes the Green function of the set A with pole at infinity. Further result on the weak* limit was given in the notion of balayage of a measure on the compact set $K := \partial V \cup (\Sigma \setminus V)$. If $K = \Sigma$, then the weak* limit of the counting measure of the zeros is the equilibrium measure on Σ.

For Sobolev inner products (7.1), asymptotic distributions of zeros of Sobolev orthogonal polynomials and their derivatives were studied in [37] in the setting that $d\mu_k(x) = x^\gamma e^{-\varphi_k(x)} dx$, where φ_k are functions having polynomial growth at infinity or iterative exponential functions, on $[0, \infty)$, which includes the Freud weights as special cases.

In another direction concerning zeros of Sobolev orthogonal products with respect to the inner product (7.2), global distribution of the zeros is related to the boundedness of the multiplication operator $f \mapsto xf$ in the norms associated with the inner product in [24]. More precisely, if this operator is bounded, that is, there exists a positive real number M such that $\langle xf, xf \rangle_S \leq M \langle f, f \rangle_S$, then the set of zeros of the Sobolev orthogonal polynomials is contained in the ball centered at the origin with radius M and the vector of measures $(d\mu_0, \ldots, d\mu_m)$ has compact support. The paper also contains other qualitative results on the zeros. Notice, however, that this approach does not give analytic properties, such as real, simple, interlacing, of the zeros.

10. Asymptotics

For ordinary orthogonal polynomials, three different types of asymptotics are considered: strong asymptotics, outer ratio asymptotics and nth root asymptotics. All three have been considered in the Sobolev setting and we summarize most relevant results in this section.

10.1. Sobolev type inner products

The first work on asymptotics for Sobolev orthogonal polynomials was carried out in [81] for the inner product

$$\langle f, g \rangle_S = \int_{-1}^{1} f(x)g(x) d\mu(x) + M_1 f'(c) g'(c),$$

where $c \in \mathbb{R}$, $M_1 > 0$ and the measure $d\mu_0$ belongs to the Nevai class $M(0, 1)$. Using the outer ratio asymptotics for the ordinary orthogonal polynomials $P_n(\cdot; d\mu_0)$ and the

connection formula between $P_n(\cdot; d\mu_0)$ and the Sobolev orthogonal polynomials S_n, as in (7.6), it was shown that, if $c \in \mathbb{R} \setminus \mathrm{supp}\mu_0$, then

$$\lim_{n\to\infty} \frac{S_n(z)}{P_n(z, d\mu_0)} = \frac{(\Phi(z) - \Phi(c))^2}{2\Phi(z)(z-c)}, \quad \Phi(z) := z + \sqrt{z^2 - 1},$$

locally uniformly outside the support of the measure, where $\sqrt{z^2 - 1} > 0$ when $z > 1$. Furthermore, if the measure belongs to the Szegő class, then the outer strong asymptotics for S_n can be deduced in a straightforward way. If $c \in \mathrm{supp}\mu_0$, then $\lim_{n\to\infty} \frac{S_n(z)}{P_n(z; d\mu_0)} = 1$ outside the support of the measure. By comparing the corresponding polynomials, such results can be deduced in a similar manner if a mass point is added to the measure.

The first extension of the above results was carried out in [6] for the Sobolev inner product (9.1) with a 2×2 matrix A. Under the same conditions on the measure, it was proved that

$$\lim_{n\to\infty} \frac{S_n(z)}{P_n(z, d\mu_0)} = \left(\frac{(\Phi(z) - \Phi(c))^2}{2\Phi(z)(z-c)} \right)^r, \quad r := \mathrm{rank}\, A,$$

locally uniformly outside the support of the measure. The second extension appears in [70] for the inner product

$$\langle f, g \rangle = \int f(x)g(x)d\mu_0(x) + \sum_{j=1}^{N} \sum_{k=0}^{N_j} f^{(k)}(c_j) L_{j,k}(g; c_j),$$

where $d\mu_0 \in M(0, 1)$, $\{c_k\}_{k=1}^{N}$ are real numbers located outside the support of the measure, and $L_{j,k}(g; c_j)$ is the evaluation at c_j of the ordinary differential operator $L_{j,k}$ acting on g such that L_{j,N_j} is not identically zero for $j = 1, 2, \ldots, N$. Assuming that the inner product is quasi-definite so that a sequence of orthogonal polynomials exist, then on every compact subset in $\mathbb{C} \setminus \mathrm{supp}d\mu_0$,

$$\lim_{n\to\infty} \frac{S_n^{(\nu)}(z)}{P_n^{(\nu)}(z, d\mu_0)} = \prod_{j=1}^{m} \left(\frac{(\Phi(z) - \Phi(c))^2}{2\Phi(z)(z-c)} \right)^{I_j},$$

where I_j is the dimension of the square matrix obtained from the matrix of the coefficients of L_{j,N_j} after deleting all zero rows and columns. The key idea for the proof is to reduce the Sobolev orthogonality in this setting to ordinary quasi-orthogonality, so that the polynomial $S_n(x)$ can be expressed as a short linear combination of polynomials $P_m(x; d\mu_0)$ and then consider the behavior of the coefficients in the linear combination.

If both the measure $d\mu_0$ and its support Δ are regular, then techniques from potential theory were used in [71] to derive the nth root asymptotics of the Sobolev orthogonal polynomials,

$$\limsup_{n\to\infty} \|S_n^{(j)}\|_\Delta^{1/n} = C(\Delta), \quad j \geq 0,$$

where $\| \cdot \|_\Delta$ denotes the uniform norm in the support of the measure and $C(\Delta)$ is its logarithmic capacity.

When the support of the measure in the inner product (9.1) is unbounded, the analysis has been focused on the case of the Laguerre weight function. The first study in [11] considered the case that $c = 0$ and A is a 2×2 diagonal matrix (see also [74] for a survey on the unbounded case). Assuming that the leading coefficient of S_n is normalized to be $\frac{(-1)^n}{n!}$, the following results on the asymptotic behavior of S_n were established:

(1) (Outer relative asymptotics) $\lim_{n \to \infty} \frac{S_n(z)}{L_n^{(\alpha)}(z)} = 1$ uniformly on compact subsets of the exterior of the positive real semiaxis.
(2) (Outer relative asymptotics for scaled polynomials) $\lim_{n \to \infty} \frac{S_n(nz)}{L_n^{(\alpha)}(nz)} = 1$ uniformly on compact subsets of the exterior of $[0, 4]$.
(3) (Mehler–Heine formula) $\lim_{n \to \infty} \frac{S_n(z/n)}{n^\alpha} = z^{-\alpha/2} J_{\alpha+4}(2\sqrt{z})$ uniformly on compact subsets of the complex plane, assuming that $\operatorname{rank} A = 2$.
(4) (Inner strong asymptotics)

$$\frac{S_n(x)}{n^{\alpha/2}} = c_3(n) e^{x/2} x^{-\alpha/2} J_{\alpha+4}\left(2\sqrt{(n-2)x}\right) + O\left(n^{-\min\{\alpha+5/4, 3/4\}}\right)$$

on compact subsets of the positive real semiaxis, where $\lim_{n \to \infty} c_3(n) = 1$.

The case that $\operatorname{rank} A = 1$ is also studied, we only state the results when A has full rank for sake of simplicity. Finally, if the point c is a negative real number, then the following outer relative asymptotics was established in [82],

$$\lim_{n \to \infty} \frac{S_n(z)}{L_n^{(\alpha)}(z)} = \left(\frac{\sqrt{-z} - \sqrt{-c}}{\sqrt{-z} + \sqrt{-c}}\right)^r, \quad r = \operatorname{rank} A,$$

uniformly on compact subsets of the exterior of the real positive semiaxis.

When $c = 0$ and A is a non-singular diagonal matrix of size $m + 1$, the following asymptotic properties of the Sobolev orthogonal polynomials with respect to the inner product (9.1) were obtained in [7],

(1) (Outer relative asymptotics) For every $\nu \in \mathbb{N}$, $\lim_{n \to \infty} \frac{S_n^{(\nu)}(z)}{(L_n^{(\alpha)})^{(\nu)}(z)} = 1$ uniformly on compact subsets of the exterior of the positive real semiaxis.
(2) (Mehler–Heine formula) $\lim_{n \to \infty} \frac{(-1)^n}{n!} \frac{S_n(z/n)}{n^\alpha} = (-1)^{m+1} z^{-\alpha/2} J_{\alpha+2m+2}(2\sqrt{z})$ uniformly on compact subsets of the complex plane.

It should be pointed out that the above Mehler–Heine formula cannot be directly deduced from the connection formula (7.6). As an interesting consequence of the Mehler–Heine formula and the Hurwitz Theorem, the local behavior of zeros of these Sobolev orthogonal polynomials can be deduced.

10.2. Continuous Sobolev inner products

We first consider the case of coherent pairs. Let $\{\mu_0, \mu_1\}$ be a coherent pair of measures and $\operatorname{supp} \mu_0 = [-1, 1]$. Then the outer relative asymptotic relation for the Sobolev orthogonal polynomials with respect to (9.2) in terms of orthogonal polynomials $P_n(\cdot; d\mu_1)$ is [87]

$$\lim_{n \to \infty} \frac{S_n(z)}{P_n(z; d\mu_1)} = \frac{2}{\Phi'(z)}, \quad \Phi(z) := z + \sqrt{z^2 - 1},$$

where $\sqrt{z^2 - 1} > 0$ when $z > 1$, uniformly on compact subsets of the exterior of the interval $[-1, 1]$. The key idea of the proof is to show that the coefficient $b_n(\lambda)$ in (5.5) satisfies $\lim_{n\to\infty} b_n(\lambda) = 0$, which is a consequence of the inequality

$$\pi_n + \lambda n^2 \tau_{n-1} \leq \|S_n(\cdot, \lambda)\|_\lambda^2 \leq \pi_n + \hat{a}_{n-1}^2 \pi_{n-1} + \lambda n^2 \tau_{n-1},$$

where $\pi_n := \|P_n(\cdot, d\mu_0)\|_{d\mu_0}^2$ and $\tau_n := \|P_n(\cdot, d\mu_1)\|_{d\mu_1}^2$, on the weighted L^2 norms.

When the measures μ_0 and μ_1 are absolutely continuous and belong to the Szegő class, the Bernstein–Szegő theory is applied in [85] to derive the outer relative asymptotics $\lim_{n\to\infty} \frac{S_n(z)}{P_n(z, d\mu_1)} = \frac{2}{\Phi'(z)}$ locally uniformly outside $[-1, 1]$. As a straightforward consequence, the strong outer asymptotics follows. If μ_0 is any finite Borel measure supported in $[-1, 1]$ in [85], then the outer relative asymptotics $\lim_{n\to\infty} \frac{S_n'(z)}{n P_{n-1}(z, d\mu_1)} = 1$ holds, which illustrates the role of the measure involved in the nonstandard part of the Sobolev inner product.

An extension of the above results for the inner product (7.2) was carried out in [88], where $d\mu_m$ is assumed to be absolutely continuous and belongs to the Szegő class, whereas other measures are assumed to be positive and supported in $[-1, 1]$. When the supports of the measures involved in the Sobolev inner product satisfy certain nesting property and the measure $d\mu_0$ is regular, the n-root asymptotic behavior is established. More specifically, for every nonnegative integer number j,

(1) $\limsup_{n\to\infty} |S_n^{(j)}(z)|^{1/n} = C(\Delta)e^{g_\Delta(z,\infty)}$ for every $z \in \mathbb{C}$ up to a set of capacity zero;
(2) $\lim_{n\to\infty} |S_n^{(j)}(z)|^{1/n} = C(\Delta)e^{g_\Delta(z,\infty)}$ uniformly on each compact subset of the complex plane outside the disk centered at the origin with radius defined in terms of the Sobolev norm of the multiplication operator,

where $g_\Delta(0, \infty)$ is the Green function of Δ with the infinite as a pole [71].

For measures of coherent pairs that have unbounded support, asymptotic properties of the corresponding Sobolev orthogonal polynomials have been extensively studied in the literature (see [74] for an overview). The outer relative asymptotics, the scaled outer asymptotics as well as the inner strong asymptotics of such polynomials have been considered for all families of coherent pairs and symmetrically coherent pairs. It should be pointed out that the outer relative asymptotics involves the parameter λ in the inner product (5.1), which does not appear in the case of bounded supports. Nevertheless, the technicalities in the unbounded case are similar to those in the bounded case, the main difficulty is on estimates for the coefficients that appear in the relations between Sobolev and ordinary orthogonal polynomials.

For instance, in the case of symmetrically coherent Hermite case, that is, when either $d\mu_0 = e^{-x^2}$ and $d\mu_1 = \frac{1}{x^2 + \xi^2} e^{-x^2}$ or $d\mu_0 = x^2 + \xi^2 e^{-x^2}$ and $d\mu_1 = e^{-x^2}$, it holds, respectively,

(1) $\lim_{n\to\infty} \frac{S_n(z,\lambda)}{H_n(z)} = \theta(\lambda)$ uniformly on compact subsets outside the real line;
(2) $\lim_{n\to\infty} \lfloor \frac{n}{2} \rfloor^{1/2} \frac{S_n(z,\lambda)}{H_n(z)} = \theta(\lambda)(\mp z + |\xi|)$, if $z \in \mathbb{C}_\pm$, uniformly on compact subsets of the half planes $\mathbb{C}_\pm = \{x \pm iy, y > 0\}$, respectively,

where $\theta(\lambda) := \frac{\Phi(2\lambda+1)}{\Phi(2\lambda+1)-1}$, as shown in [74].

The case $d\mu_0 = d\mu_1 = e^{-x^4}$ of the inner product (5.1), or the $(2, 0)$ self-coherent pair with Freud weight, was studied in [21], where the connection between Sobolev and ordinary orthogonal polynomials is given by $P_n(x; d\mu) = S_n(x; \lambda) + c_{n-2}(\lambda)S_{n-2}(x; \lambda)$. In order to deduce its outer relative asymptotics, it is necessary to estimate the values of $c_n(\lambda)$ for n sufficiently large. It turns out that $\lim_{n\to\infty} n^{-1/2}c_n(\lambda) = \frac{1}{6\sqrt{3}}$, which leads to, in a straightforward way, $\lim_{n\to\infty} \frac{S_n(z,\lambda)}{P_n(z,d\mu_0)} = \frac{3}{2}$ uniformly on compact subsets outside the real line. The outer relative asymptotics, with appropriate scaling, was also obtained in [21], taking into account the Rakhmanov–Mhaskar–Saff constant for these Freud polynomials.

For asymptotics, few examples of generalized coherent pairs of measures have been considered in the literature. The Freud–Sobolev case considered above motivated further study of Sobolev inner products with exponential weights. Let $W(x) = e^{-Q(x)}$, where Q is a continuous even function in $\mathbb{R}$ such that Q'' is continuous in $(0, \infty)$ and $Q' > 0$ in $(0, \infty)$, and $\alpha \leq \frac{xQ''(x)}{Q'(x)} \leq \beta$ for some $\beta > \alpha > 0$. The asymptotic behavior of Sobolev orthogonal polynomials for the inner product (9.2) with $d\mu_0(x) = (\psi(x)W(x))^2 dx$ and $d\mu_1(x) = \lambda W^2(x)dx$, where $\psi \in L_\infty(\mathbb{R})$, was studied in [47]. The derivative of the orthonormal Sobolev polynomials s_n behaves as $\lambda^{-1/2}p_{n-1}(.; W^2)$, the orthonormal polynomials with respect to the measure $W^2(x)dx$, in the sense of the L_2 asymptotics, that is, $\|s'_n(\cdot) - \lambda^{-1/2}p_{n-1}(\cdot; W^2)\|_{W^2 dx} = O(\frac{a_n}{n})$, where a_n is the Mhaskar–Rakhmanov–Saff number for Q. On the other hand, a uniform bound for the corresponding scaled polynomials is also deduced with the help of a simple Nikolskii inequality. As in the bounded case, the measure $d\mu_1$ plays a key role in the asymptotic behavior of the Sobolev orthonormal polynomials.

11. Sobolev orthogonal polynomials of several variables

In contrast to one variable, Sobolev orthogonal polynomials of several variables are studied only recently. In this section we report what has been done in this direction.

11.1. Orthogonal polynomials of several variables

For $x \in \mathbb{R}^d$ and $\alpha \in \mathbb{N}_0^d$, the (total) degree of the monomial x^α is, by definition, $|\alpha| := \alpha_1 + \cdots + \alpha_d$. Let Π_n^d denote the space of polynomials of total degree at most n in d-variables. It is known that $\dim \Pi_n^d = \binom{n+d}{n}$. Let Π^d denote the space of all polynomials in d-variables. Let $\langle \cdot, \cdot \rangle$ be an inner product defined on $\Pi^d \times \Pi^d$. A polynomial $P \in \Pi_n^d$ is orthogonal if $\langle P, q \rangle = 0$ for all $q \in \Pi_{n-1}^d$. For $n \in \mathbb{N}_0^d$, let $\mathcal{V}_n^d$ denote the space of polynomials of total degree n. Then $\dim \mathcal{V}_n^d = \binom{n+d-1}{n}$. In contrast to one-variable, the space $\mathcal{V}_n^d$ can have many different bases when $d \geq 2$. Moreover, the elements in $\mathcal{V}_n^d$ may not be orthogonal to each other.

For the structure and properties of orthogonal polynomials in several variables, we refer to [38]. In the following, we describe briefly two families of orthogonal polynomials as examples.

Example 1. For $i = 1, 2$, let w_i be weight functions defined on an interval $[a_i, b_i]$ of the real line and let $p_n(w_i; \cdot)$ be the orthogonal polynomial of degree n with respect to w_i. With respect to the weight function $W(x, y) := w(x)w(y)$ on $[a_1, b_1] \times [a_2, b_2]$, one family of mutually orthogonal basis of $\mathcal{V}_n^2(W)$ is given by

$$P_k^n(x, y) = p_k(w_1; x) p_{n-k}(w_2; y), \quad 0 \le k \le n. \tag{11.1}$$

Because Π_n^d is defined in terms of total degree, which is different from the tensor product $\Pi_n \times \Pi_n$, every element of $\mathcal{V}_n^2$ is of total degree n.

For our second example, we need the definition of spherical harmonics. Let $\mathcal{P}_n^d$ denote the space of homogeneous polynomials of degree n in d-variables. A polynomial Y is a spherical harmonic of degree n if $Y \in \mathcal{P}_n^d \cap \ker \Delta$, where Δ is the Laplacian operator, $\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}$. Let $\mathcal{H}_n^d$ denote the space of spherical harmonics of degree n. It is known that

$$a_n^d := \dim \mathcal{H}_n^d = \binom{n+d-1}{n} - \binom{n+d-3}{n-2}.$$

The elements of $\mathcal{H}_n^d$ are orthogonal to lower degree polynomials with respect to the inner product

$$\langle f, g \rangle_{\mathbb{S}^{d-1}} := \int_{\mathbb{S}^{d-1}} f(\xi) g(\xi) d\sigma(\xi),$$

where $d\sigma$ denotes the surface measure on $\mathbb{S}^{d-1}$. An orthonormal basis can be constructed explicitly in terms of the Gegenbauer polynomials in spherical coordinates. For properties of harmonic polynomials and their relations to orthogonal polynomials, we refer to [27,38] and references therein.

Example 2. For $\mu > -1$, let $\varpi_\mu(x) = (1 - \|x\|^2)^{\mu - 1/2}$ be the weight function defined on the unit ball $\mathbb{B}^d = \{x \in \mathbb{R}^d : \|x\| \le 1\}$, where $\|x\|$ denotes the Euclidean norm of $x \in \mathbb{R}^d$. Orthogonal polynomials with respect to ϖ_μ can be given in several different formulations. We give one basis of $\mathcal{V}_n^d(\varpi_\mu)$ in terms of the Jacobi polynomials and spherical harmonics in the spherical coordinates $x = r\xi$, where $0 < r \le 1$ and $\xi \in \mathbb{S}^{d-1} = \{x : \|x\| = 1\}$. For $0 \le j \le n/2$ and $1 \le j \le a_{n-2j}^d$, define

$$P_{j,\nu}^n(x) := P_j^{(\mu, n-2j+\frac{d-2}{2})}(2\|x\|^2 - 1) Y_\nu^{n-2j}(x), \tag{11.2}$$

where $\{Y_\nu^{n-2j} : 1 \le \nu \le a_{n-2j}^d\}$ is an orthonormal basis of $\mathcal{H}_{n-2j}^d$. Then the set $\{P_{j,\ell}^{\mu,n}(x) : 0 \le j \le \frac{n}{2}, 1 \le \ell \le a_{n-2j}^d\}$ is a mutually orthogonal basis of $\mathcal{V}_n^d(\varpi_\mu)$. The elements of $\mathcal{V}_n^d$ are eigenfunctions of a second order differential operator $\mathcal{D}_\mu$. More precisely, we have

$$\mathcal{D}_\mu P = -(n+d)(n+2\mu)P, \quad \forall P \in \mathcal{V}_n^d(\varpi_\mu), \tag{11.3}$$

where

$$\mathcal{D}_\mu := \Delta - \sum_{j=1}^d \frac{\partial}{\partial x_j} x_j \left[2\mu + \sum_{i=1}^d x_i \frac{\partial}{\partial x_i} \right].$$

11.2. Sobolev orthogonal polynomials on the unit ball

At the moment of this writing, we know more about Sobolev orthogonal polynomials on the unit ball than on any other domain.

The first work in this direction deals with the inner product [102]

$$\langle f, g \rangle_\Delta := \int_{\mathbb{B}^d} \Delta \Big[(1 - \|x\|^2) f(x) \Big] \Delta \Big[(1 - \|x\|^2) g(x) \Big] dx,$$

which arises from the numerical solution of the Poisson equation [12]. The geometry of the ball and (11.2) suggests that one can look for a mutually orthogonal basis of the form

$$q_j(2\|x\|^2 - 1) Y_\nu^{n-2j}(x), \quad Y_\nu^{n-2j} \in \mathcal{H}_{n-2j}^d, \tag{11.4}$$

where q_j is a polynomial of degree j in one variable. Such a basis was constructed in [102] for the space $\mathcal{V}_n^d(\Delta)$ with respect to $\langle \cdot, \cdot \rangle_\Delta$. As a result, it was shown that

$$\mathcal{V}_n^d(\Delta) = \mathcal{H}_n^d \oplus (1 - \|x\|^2) \mathcal{V}_{n-2}(\varpi_2).$$

The next inner product considered on the ball, which should be, in retrospect, the first one being considered, is defined by

$$\langle f, g \rangle_{-1} := \lambda \int_{\mathbb{B}^d} \nabla f(x) \cdot \nabla g(x) dx + \int_{\mathbb{S}^{d-1}} f(\xi) g(\xi) d\sigma(\xi),$$

where $\lambda > 0$. An alternative is to replace the integral over $\mathbb{S}^{d-1}$ by $f(0)g(0)$. A basis of the form (11.4) was constructed explicitly in [103] for the space $\mathcal{V}_n^d(\Delta)$ with respect to $\langle \cdot, \cdot \rangle_{-1}$, from which it follows that

$$\mathcal{V}_n^d(\varpi_{-1}) = \mathcal{H}_n^d \oplus (1 - \|x\|^2) \mathcal{V}_{n-2}(\varpi_1). \tag{11.5}$$

The main part of the base, those in $(1 - \|x\|^2) \mathcal{V}_{n-2}(\varpi_1)$, can be given in terms of the Jacobi polynomials $P_n^{(-1,b)}$ of negative index, which explains why we used the notation ϖ_{-1}. Another interesting aspect of this case is that the polynomials in $\mathcal{V}_n^d(\varpi_{-1})$ are eigenfunctions of the differential operator $\mathcal{D}_{-1}$, the limiting case of (11.3).

For $k \in \mathbb{N}$, the equation $\mathcal{D}_{-k} Y = \lambda_n Y$ of (11.3) was studied in [97], where a complete system of polynomial solutions was determined explicitly. For $k \geq 2$, however, it is not known if the solutions are Sobolev orthogonal polynomials. Closely related to the case of $k = 2$ is the following inner product

$$\langle f, g \rangle_{-2} := \lambda \int_{B^d} \Delta f(x) \Delta g(x) dx + \int_{S^{d-1}} f(x) g(x) d\sigma, \quad \lambda > 0.$$

An explicit basis for the space $\mathcal{V}_n^d(\varpi_{-2})$ of the Sobolev orthogonal polynomials with respect to $\langle \cdot, \cdot \rangle_{-2}$ was constructed in [97], from which it follows that

$$\mathcal{V}_n^d(\varpi_{-2}) = \mathcal{H}_n^d \oplus (1 - \|x\|^2) \mathcal{H}_{n-2}^d \oplus (1 - \|x\|^2)^2 \mathcal{V}_{n-4}^d(\varpi_2). \tag{11.6}$$

The main part of the base, those in $(1 - \|x\|^2)^2 \mathcal{V}_{n-2}(\varpi_2)$, can be given in terms of the Jacobi polynomials $P_n^{(-2,b)}$ of negative index.

It turns out that the Sobolev orthogonal polynomials for the last two cases can be used in the study of the spectral method for the numerical solution of partial differential equations. This connection was established in [69], where, for $s \in \mathbb{N}$, the following inner product in the Sobolev space $W_p^s(\mathbb{B}^d)$ is defined,

$$\langle f, g \rangle_{-s} := \langle \nabla^s f, \nabla^s g \rangle_{\mathbb{B}^d} + \sum_{k=0}^{\lceil \frac{\varrho}{2} \rceil - 1} \lambda_k \langle \Delta^k f, \Delta^k g \rangle_{\mathbb{S}^{d-1}}, \tag{11.7}$$

where λ_k, $k = 0, 1 \ldots, \lceil \frac{\varrho}{2} \rceil - 1$, are positive constants, and

$$\nabla^{2m} := \Delta^m \quad \text{and} \quad \nabla^{2m+1} := \nabla \Delta^m, \quad m = 1, 2, \ldots.$$

For $s > 2$, the space $\mathcal{V}_n^d(\varpi_{-s})$ associated with $\langle \cdot, \cdot \rangle_{-s}$ cannot be decomposed as in (11.5) and (11.6). Nevertheless, an explicit mutually orthogonal basis was constructed in [69], which requires considerable effort, and the basis uses extension of the Jacobi polynomials $P_n^{(\alpha,\beta)}$ for $\alpha, \beta \in \mathbb{R}$ that avoids the degree reduction when $-\alpha - \beta - n \in \{0, 1, \ldots, n\}$. The main result in [69] establishes an estimate for the polynomial approximation in the Sobolev space $\mathcal{W}_p^s(\mathbb{B}^d)$, the proof relies on the Fourier expansion in the Sobolev orthogonal polynomials associated with (11.7).

Another Sobolev inner product considered on the unit ball is defined by

$$\langle f, g \rangle = \int_{\mathbb{B}^d} \nabla f(x) \cdot \nabla g(x) W_\mu(x) dx + \lambda \int_{\mathbb{B}^d} f(x) g(x) W_\mu(x) dx,$$

which is an extension of the Sobolev inner product of the coherent pair in the case of the Gegenbauer weight of one-variable. A mutually orthogonal basis was constructed in [96], which has the form of (11.4) but the corresponding q_j is orthogonal with respect to a rather involved Sobolev inner product of one variable.

11.3. Sobolev orthogonal polynomials on the simplex

Let T^d be the simplex of $\mathbb{R}^d$ defined by

$$T^d := \{x \in \mathbb{R}^d : x_1 \geq 0, \ldots, x_d \geq 0, 1 - |x| \geq 0\},$$

where $|x| := x_1 + \cdots + x_d$. The classical weight function on T^d is defined by

$$\varpi_{\boldsymbol{\gamma}}(x) := x_1^{\gamma_1} \cdots x_d^{\gamma_d} (1 - |x|)^{\gamma_{d+1}}, \quad x \in T^d, \tag{11.8}$$

where γ_i are real numbers, usually assumed to satisfy $\gamma_i > -1$ to ensure the integrability of $\varpi_{\boldsymbol{\gamma}}$ on T^d. Let $c_{\boldsymbol{\gamma}} = 1 \big/ \int_{T^d} \varpi_{\boldsymbol{\gamma}}(x) dx$ denote the normalization constant. We consider the inner product

$$\langle f, g \rangle_{\boldsymbol{\gamma}} := c_{\boldsymbol{\gamma}} \int_{T^d} f(x) g(x) \varpi_{\boldsymbol{\gamma}}(x) dx.$$

The space $\mathcal{V}_n^d(\varpi_{\boldsymbol{\gamma}})$ of orthogonal polynomials of degree n for this inner product contains several explicit bases, which have been studied extensively (cf. [38]). One particular basis is given by the Rodrigues type formula

$$P_{\mathbf{n}}^{\boldsymbol{\gamma}}(x) := x^{-\boldsymbol{\gamma}}(1 - |x|)^{-\gamma_{d+1}} \frac{\partial^{|\mathbf{n}|}}{\partial x^{\mathbf{n}}}\left[x^{\boldsymbol{\gamma}+\mathbf{n}}(1 - |x|)^{\gamma_{d+1}+|\mathbf{n}|}\right], \tag{11.9}$$

where $\frac{\partial^{|\mathbf{n}|}}{\partial x^{\mathbf{n}}} = \frac{\partial^{|\mathbf{n}|}}{\partial x_1^{n_1} \cdots \partial x_d^{n_d}}$ and $\mathbf{n} \in \mathbb{N}_0^d$. Furthermore, it is known that polynomials in $\mathcal{V}_n^d(W_{\boldsymbol{\gamma}})$ are eigenfunctions of the differential operator

$$L_{\boldsymbol{\gamma}} P := \sum_{i=1}^d x_i(1 - x_i)\frac{\partial^2 P}{\partial x_i^2} - 2\sum_{1 \le i < j \le d} x_i x_j \frac{\partial^2 P}{\partial x_i \partial x_j}$$
$$+ \sum_{i=1}^d (\gamma_i + 1 - (|\boldsymbol{\gamma}| + d + 1)x_i)\frac{\partial P}{\partial x_i},$$

where $|\boldsymbol{\gamma}| := \gamma_1 + \cdots + \gamma_{d+1}$; more precisely,

$$L_{\boldsymbol{\gamma}} P = -n(n + |\boldsymbol{\gamma}| + d) P, \quad \forall P \in \mathcal{V}_n^d(\varpi_{\boldsymbol{\gamma}}). \tag{11.10}$$

If some or all γ_i are equal to -1, the weight function becomes singular but Eq. (11.10) still has a full set of polynomial solutions. In [1], these solutions were given explicitly and were shown to be the Sobolev orthogonal polynomials with respect to explicitly given inner products. For $d = 2$, the simplex is the triangle T^2, writing the weight function as $\varpi_{\alpha,\beta,\gamma}(x) = x^\alpha y^\beta(1 - x - y)^\gamma$, then the inner products are of the form

$$\langle f, g\rangle_{\alpha,\beta,-1} := \int_{T^2}\left[x\partial_x f(x, y)\partial_x g(x, y) + y\partial_y f(x, y)\partial_y g(x, y)\right]x^\alpha y^\beta dxdy$$
$$+ \lambda_1 \int_0^1 f(x, 1 - x)g(x, 1 - x)x^\alpha(1 - x)^\beta dx$$

$$\langle f, g\rangle_{\alpha,-1,-1} := \int_{T^2} \partial_y f(x, y)\partial_y g(x, y)x^\alpha dxdy,$$
$$+ \lambda_1 \int_0^1 \partial_x f(x, 0)\partial_x g(x, 0)x^{\alpha+1}dx + \lambda_{1,0}f(1, 0)g(1, 0)$$

$$\langle f, g\rangle_{-1,-1,-1} := \int_{T^2} \partial_{xy} f(x, y)\partial_{xy} g(x, y)(1 - x - y)dxdy,$$
$$+ \lambda_1 \int_0^1 \partial_x f(x, 0)\partial_x g(x, 0)dx + \lambda_2 \int_0^1 \partial_y f(0, y)\partial_y g(0, y)dy$$
$$+ \lambda_{1,0}f(1, 0)g(1, 0) + \lambda_{0,1}f(0, 1)g(0, 1) + \lambda_{0,0}f(0, 0)g(0, 0).$$

The first case can be deduced by taking limit $\gamma \to -1$ in the classical inner product with respect to $\varpi_{\alpha,\beta,\gamma}$, as observed in [19]. Identifying the correct form of the inner product is a major step. For $d > 2$, one needs to consider the lower dimensional faces of the simplex T^d. Fortunately, restrictions of the polynomials in (11.9) remain orthogonal polynomials on the faces.

Besides those considered in [1], no other family of Sobolev orthogonal polynomials has been studied on the simplex.

11.4. Sobolev orthogonal polynomials on product domain

On the product domain $[a_1, b_1] \times [a_2, b_2]$ of $\mathbb{R}^2$, define the product weight function

$$\varpi(x_1, x_2) = w_1(x_1)w_2(x_2),$$

where w_i is a weight function on $[a_i, b_i]$ for $i = 1, 2$. With respect to ϖ, we consider the Sobolev inner product

$$\langle f, g \rangle_S := \int_{[a,b]^2} \nabla f(x, y) \cdot \nabla g(x, y)\varpi(x, y)dxdy + \lambda f(c_1, c_2)g(c_1, c_2),$$

where $\nabla f = (\partial_x f, \partial_y g)$, $\lambda > 0$ and (c_1, c_2) is a fixed point in $\mathbb{R}^2$.

A moment reflection shows that orthogonal polynomials with respect to this inner product are no longer products as that of (11.1) in general. Two cases are considered in [43]. The first one is the product Laguerre weight for which

$$\langle f, g \rangle_S := \int_0^\infty \int_0^\infty \nabla f(x, y) \cdot \nabla g(x, y)w_\alpha(x)w_\beta(y)dxdy + \lambda_k f(0, 0)g(0, 0),$$

where $w_\alpha(x) = x^\alpha e^{-x}$. The Sobolev orthogonal polynomials are related to the polynomials $Q_{j,m}^{\alpha,\beta}$ defined by

$$Q_{j,m}^{\alpha,\beta}(x, y) := Q_{m-j}^\alpha(x)Q_j^\beta(y) \quad \text{with } Q_n^\alpha(x) := \widehat{L}_n^{(\alpha)}(x) + n\widehat{L}_{n-1}^{(\alpha)}(x),$$

where $\widehat{L}_n^{(\alpha)}$ denotes the nth monic Laguerre polynomial. The polynomial Q_n^α is monic and it satisfies $\frac{d}{dx}Q_n^\alpha(x) = n\widehat{L}_{n-1}^{(\alpha)}(x)$. For $0 \le k \le n$, let $S_{n-k,k}^{\alpha,\beta}(x, y) = x^{n-k}y^k + \cdots$ be the monic Sobolev orthogonal polynomials of degree n. Define the column vectors

$$\mathbb{Q}_n^{\alpha,\beta} := (Q_{0,n}^{\alpha,\beta}, \ldots, Q_{n,n}^{\alpha,\beta})^T \quad \text{and} \quad \mathbb{S}_n^{\alpha,\beta} := (S_{0,n}^{\alpha,\beta}, \ldots, S_{n,n}^{\alpha,\beta})^T.$$

It was shown in [43] that there is a matrix B_{n-1} such that

$$\mathbb{Q}_n^{\alpha,\beta} = \mathbb{S}_n^{\alpha,\beta} + B_{n-1}\mathbb{S}_{n-1}^{\alpha,\beta}$$

and the matrix B_{n-1} and the norm $\langle \mathbb{S}_n^{\alpha,\beta}, \mathbb{S}_n^{\alpha,\beta} \rangle_S$ can both be computed by one recursive algorithm.

The above construction of orthogonal basis for the product domain works if w_1 and w_2 are self-coherent. The case that both are the Gegenbauer weight functions was given as a second example in [43].

11.5. Miscellaneous results

Sobolev orthogonal polynomials in two variables that satisfy second order partial differential equations are discussed in [66]. The paper, however, contains few concrete examples.

In [52], a large family of commutative algebras of partial differential operators invariant under rotations, called Krall–Jacobi algebra, is constructed and analyzed. The study leads naturally to the Sobolev orthogonal polynomials with respect to an inner product on the unit ball that involves spherical Laplacian.

For inner product that contains additional point evaluations of functions, as those discussed in Section 7, the Krall type construction of orthogonal polynomials can be extended to several variables, as shown in [33]. The same holds true if the point evaluations involve derivatives, see [35] for an example.

12. Orthogonal expansions in Sobolev orthogonal polynomials

Let $\{p_n\}_{n \geq 0}$ be a system of orthogonal polynomials with respect to an inner product $\langle \cdot, \cdot \rangle$. The Fourier orthogonal expansion of a function f in $\{p_n\}_{n \geq 0}$ is defined by

$$f(x) \sim \sum_{n=0}^{\infty} \widehat{f}_n p_n(x), \quad \widehat{f}_n = \frac{1}{\sqrt{\langle p_n, p_n \rangle}} \langle f, p_n \rangle.$$

The nth partial sum $S_n f$ if defined by

$$S_n f(x) := \sum_{k=0}^{n} \widehat{f}_k p_k(x) = \langle f, K_n(x, \cdot) \rangle,$$

where $K_n(\cdot, \cdot)$ is the reproducing kernel of the space of polynomials of degree at most n, defined by

$$K_n(x, y) = \sum_{k=0}^{n} \frac{1}{\langle p_k, p_k \rangle} p_k(x) p_k(y).$$

The Fourier expansions in terms of classical orthogonal polynomials have been studied extensively in the literature. One of the essential tools is the Christoffel–Darboux formula, which gives a closed formula for the kernel $K_n(\cdot, \cdot)$. For Sobolev orthogonal polynomials, however, the Christoffel–Darboux formula no longer holds, which impedes the study of the Fourier expansion in Sobolev orthogonal polynomials through standard techniques. Indeed, except one class of Sobolev orthogonal polynomials, little has been done in this direction.

The exceptional class is tied with applications in the spectral methods for solving differential equations. Approximations using orthogonal expansions in Sobolev spaces have been extensively studied by spectral methods community; see, for example, [23] and numerous books (for example, [18,22,51]) on the subject, although Sobolev orthogonal polynomials are not often used or used only implicitly. As an example of the exceptional class, consider the inner product

$$\langle f, g \rangle_{-s} := \int_{-1}^{1} f^{(s)}(x) g^{(s)}(x) dx + \sum_{j=0}^{s-1} \lambda_j [f^{(j)}(1) + f^{(-1)}(-1)].$$

The orthogonal polynomials with respect to this inner product have been used implicitly in the spectral method; see, for example, [50,49,100]. The error estimate for the spectral method requires estimating the error of polynomial approximation in the Sobolev space

$W_2^s[-1, 1]$. By subtracting a polynomial $g \in \Pi_{2s-1}$ that satisfies $g^{(j)}(1) = g^{(j)}(-1) = 0$ for $j = 0, 1, \ldots, m - 1$, we can assume that f vanishes on the boundary terms. Let $S_n^{-s} f$ and S_n^0 denote the nth partial sum of the Fourier expansion of f in terms of the Sobolev orthogonal polynomials and the Legendre polynomials $P_n^{(0,0)}$, respectively. It is not difficult to see that $\partial^s S_n^{-s} f = S_{n-s}^0 \partial^s f$, which implies that $\partial^s (f - S_n^{-s}) = \partial^s f - S_{n-s}^0(\partial^s f)$. Thus, the estimate for the highest order derivative in W_2^s follows from the estimate of the derivative of f in the usual L^2 norm. The estimate that the spectral method requires is of the form

$$\|f - p_n\|_{W_2^s} \le cn^{-r+s}\|f\|_{W_2^r}, \quad r \ge s,$$

where p_n is a polynomial of degree n. Under the name of simultaneous approximation, an inequality of this type has also been established in approximation theory for W_p^s with $1 \le p < \infty$; see, for example, [61]. Such results can also be established for the inner product with the Jacobi weight function (see [100] and the references therein).

In the same spirit, spectral approximation on the unit ball was studied in [69], where the Sobolev orthogonal polynomials associated with (11.7) play an essential role. In contrast to one variable, we can no longer construct a polynomial g of low degree so that $f - g$ vanishes on the boundary and, as a result, the analysis in [69] is more involved.

Besides the above class, little has been established for Fourier expansions in other Sobolev orthogonal polynomials. For the Legendre–Sobolev inner product

$$\langle f, g \rangle_\lambda = \int_{-1}^{1} f(x)g(x)dx + \lambda \int_{-1}^{1} f'(x)g'(x)dx, \quad \lambda \ge 0,$$

which is (3.1) and the first Sobolev inner product ever studied, it was observed in [55], based on computational evidence, that the Fourier expansion in the Sobolev orthogonal polynomials behaviors markedly better than the Fourier expansion in the Legendre toward the end point of the interval. Similar phenomenon was also observed in later papers on Sobolev orthogonal polynomials associated with measures that are coherent pairs, see [30] and the references therein. It should be mentioned that computation of Sobolev orthogonal polynomials is discussed in [44,46], where several algorithms are provided. From a heuristic point of view, Sobolev orthogonal expansions should have a better approximation behavior than ordinary orthogonal expansions, as the former requires more information on the function being expanded. However, at the time of this writing, there has been no theoretical result that either prove or quantify that this is indeed the case.

For approximation in Sobolev spaces, it is to be expected that one should use Sobolev orthogonality instead of ordinary orthogonality. Given the amount of works that have been carried out over years, it is surprising how little has been done on the Fourier expansions in Sobolev orthogonal polynomials. As discussed in Section 2, the initial motivation for studying Sobolev orthogonal polynomials came from the problem of least square approximation in Sobolev spaces. We have gained substantial knowledge on the Sobolev orthogonality, it is now time to go back to the beginning, studying the Fourier expansions and approximation by polynomials in Sobolev spaces, and to find connections and apply what we have learnt to solve problems in other fields. We end this survey with this call of action.

Acknowledgments

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