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Exceptional Orthogonal Polynomials via Krall Discrete Polynomials

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Abstract: We consider two important extensions of the classical and classical discrete orthogonal polynomials: namely, Krall and exceptional polynomials. We also explore the relationship between both extensions and how they can be used to expand the Askey tableau.

Introduction

In these lectures, we will consider two important extensions of the classical and classical discrete orthogonal polynomials: namely, Krall and exceptional polynomials. On the one hand, Krall or bispectral polynomials are orthogonal polynomials that are also common eigenfunctions of higher-order differential or difference operators. On the other hand, exceptional polynomials have recently appeared in connection with quantum mechanical models associated to certain rational perturbations of classical potentials. We also explore the relationship between both extensions and how they can be used to expand the Askey tableau.

Section 1.1. *Background on classical and classical discrete polynomials.* The explicit solution of certain mathematical models of physical interest often depends on the use of special functions. In many cases, these special functions turn out to be certain families of orthogonal polynomials which, in addition, are also eigenfunctions of second-order operators of some specific kind. We can consider these families as the workhorse of all classical mathematical physics, ranging from potential theory, electromagnetism, etc. through the successes of quantum mechanics in the 1920s in the hands of Schrödinger. These families are called "classical orthogonal polynomials". E.J. Routh proved in 1884 (see [77]) that the only families of orthogonal polynomials (with respect to a positive weight) that can be simultaneous eigenfunctions of a second-order differential operator are those going with the names of Hermite, Laguerre and Jacobi. This result is also a consequence of the Bochner classification theorem of 1929 [7]. The similar question for second-order difference operators gave rise to the classical discrete families of orthogonal polynomials (Charlier, Meixner, Krawtchouk, Hahn), classified by Lancaster in 1941 [61]. Finally, second-order q-difference operators gave rise to the q-classical families of orthogonal polynomials (Askey–Wilson, q-Racah, etc.), although the q-families will not be considered in these lectures.

Sections 1.2, 1.3 and 1.4. *The Askey tableau. Constructing Krall and Krall discrete orthogonal polynomials using $\mathcal{D}$-operators.*

Since all these families of orthogonal polynomials can be represented by hypergeometric functions, they are also known as hypergeometric orthogonal polynomials, and they are organized as a hierarchy in the so-called Askey tableau.

As an extension of the classical families, more than 75 years ago the first families of orthogonal polynomials which are also eigenfunctions of higher-order differential operators were discovered by H.L. Krall, who classified orthogonal polynomials which are also eigenfunctions of differential operators of order 4. Because of that, orthogonal polynomials which are eigenfunctions of differential or difference operators of higher order are usually called Krall polynomials and Krall discrete polynomials, respectively. Following the terminology of Duistermaat and Grünbaum (see [11]), they are also called bispectral, and this is because of the following reason. In the continuous parameter, they are eigenfunctions of the above-mentioned operators, and in the discrete parameter, they are eigenfunctions of a second-order difference operator: the three-term recurrence relation (which is equivalent to orthogonality with respect to a measure supported in the real line).

Since the 1980s, a lot of effort has been devoted to studying Krall polynomials, with contributions by L.L. Littlejohn, A.M. Krall, J. Koekoek and R. Koekoek. A. Grünbaum and L. Haine (and collaborators), K. H. Kwon (and collaborators), A. Zhedanov, P. Iliev, and many others. The orthogonality of all these families is with respect to particular cases of Laguerre and Jacobi weights together with one or several Dirac deltas (and its derivatives) at the end points of their interval of orthogonality.

Surprisingly enough, until very recently no example was known in the case of difference operators, despite the problem being explicitly posed by Richard Askey in 1990, more than twenty five years ago. The results known for the continuous case do not provide enough help: indeed, adding Dirac deltas to the classical discrete weights does not seem to work. The first examples of Krall discrete polynomials appeared three years ago in a paper of mine, where I proposed some conjectures on how to construct Krall discrete polynomials by multiplying the classical discrete weights by the "annihilator polynomial" of certain finite sets of numbers. These conjectures have been already proved by using a new concept: $\mathscr{D}$-operators. $\mathscr{D}$-operators provide a unified approach to construct Krall, Krall discrete or q-Krall orthogonal polynomials.

This approach has also led to the discovery of new and deep symmetries for determinants whose entries are classical and classical discrete orthogonal polynomials, and has led to an unexpected connection of these symmetries with Selberg type formulas and constant term identities.

Sections 1.5 and 1.6. *Exceptional orthogonal polynomials. The dual connection with Krall polynomials at the discrete level. Expanding the Askey tableau.*

Exceptional orthogonal polynomials are complete orthogonal polynomial systems with respect to a positive measure which in addition are eigenfunctions of a second-order differential operator. They extend the classical families of Hermite, Laguerre and Jacobi.

The most apparent difference between classical orthogonal polynomials and exceptional orthogonal polynomials is that the exceptional families have a finite number of gaps in their degrees. That is, not all degrees are present in the sequence of polynomials (as it happens with the classical families). Besides that, they form a complete orthonormal set in the underlying Hilbert space defined by the orthogonalizing positive measure.

This means in particular that they are not covered by the hypotheses of Bochner's classification theorem. Each family of exceptional polynomials is associated to a quantum-mechanical potential whose spectrum and eigenfunctions can be calculated using the exceptional family. These potentials turn out to be, in each case, a rational perturbation of the classical potentials associated to the classical polynomials. Exceptional orthogonal polynomials have been applied to shape-invariant potentials, supersymmetric transformations, discrete quantum mechanics, mass-dependent potentials, and quasi-exact solvability. Exceptional polynomials appeared some nine years ago, but there has been a remarkable activity around them mainly by theoretical physicists (with contributions by D. Gómez-Ullate,

N. Kamran and R. Milson, Y. Grandati, C. Quesne, S. Odake and R. Sasaki, and many others).

In the same way, exceptional discrete orthogonal polynomials are an extension of discrete classical families such as Charlier, Meixner, Krawtchouk and Hahn. They are complete orthogonal polynomial systems with respect to a positive measure (but having gaps in their degrees) which in addition are eigenfunctions of a second-order difference operator.

Taking into account these definitions, it is scarcely surprising that no connection has been found between Krall and exceptional polynomials. However, if one considers Krall discrete polynomials, something very exciting happens: duality (roughly speaking, swapping the variable with the index) interchanges Krall discrete and exceptional discrete polynomials. This unexpected connection of Krall discrete and exceptional polynomials allows a natural and important extension of the Askey tableau. Also, this worthy fact can be used to solve some of the most interesting questions concerning exceptional polynomials; for instance, to find necessary and sufficient conditions such that the associated second-order differential operators do not have any singularity in their domain. This important issue is very much related to the existence of an orthogonalizing measure for the corresponding family of exceptional polynomials.

1.1 The classical and classical discrete families

1.1.1 Weights on the real line

These lectures deal with some relevant examples of orthogonal polynomials. Orthogonality here is with respect to the inner product defined by a weight in the linear space of polynomials with real coefficients (which we will denote by $\mathbb{R}[x]$).

Definition 1.1 A weight μ is a positive Borel measure with support in the real line satisfying

(1) μ has finite moments of every order: i.e., the integrals $\int x^n d\mu(x)$ are finite for $n \in \mathbb{N} := \{0,1,2,\dots\}$;
(2) μ has infinitely many points in its support (x is in the support of μ if $\mu(x-\varepsilon, x+\varepsilon) > 0$ for all $\varepsilon > 0$).

Condition (2) above is equivalent to saying that

$$\int p^2(x) d\mu(x) > 0, \quad \text{for } p \in \mathbb{R}[x],\ p \neq 0. \tag{1.1}$$

We associate to the weight μ the inner product defined in $\mathbb{R}[x]$ by

$$\langle p,q\rangle_\mu = \int p(x)q(x)d\mu(x). \tag{1.2}$$

By applying the Gram–Schmidt orthogonalization process to the sequence $1, x, x^2, x^3, \dots$ (condition (1.1) is required), one can generate a sequence $(p_n)_n$, $n = 0,1,2,3,\dots$, of polynomials with $\deg p_n = n$ that satisfy the orthogonality condition

$$\int p_n(x)p_m(x)d\mu(x) = c_n\delta_{n,m}, \quad c_n > 0.$$

We then say that the polynomial sequence $(p_n)_n$ is orthogonal with respect to the weight μ. When $c_n = 1$, we say that the polynomial p_n is orthonormal. It is not difficult to see that the orthogonal polynomial p_n is unique up to multiplicative constants.

Except for multiplicative constants, the nth orthogonal polynomial p_n is characterized because $\int p_n(x)q(x)d\mu(x) = 0$ for $q \in \mathbb{R}[x]$ with $\deg q \leq n-1$. This is trivially equivalent to saying that $\int p_n(x)x^k d\mu(x) = 0$ for $0 \leq k \leq n-1$.

Condition (2) above can be weakened; if we assume that the positive measure μ has N points in its support (say, x_i, $1 \leq i \leq N$), with $N < \infty$, we can only guarantee the existence of N orthogonal polynomials p_n, $n = 0,1,\dots,N-1$, with respect to μ. Indeed, up to multiplicative constants, the polynomial $p(x) = \prod_{i=1}^N (x-x_i)$ is the only one with degree N orthogonal to p_n, $n = 0,1,\dots,N-1$. But the norm of p is zero.

1.1.2 The three-term recurrence relation

Orthogonality with respect to a weight can be characterized in terms of an algebraic equation. Indeed, since xp_n is a polynomial of degree $n+1$, we can expand it in terms of the polynomials $p_0, p_1, \dots, p_{n+1}$:

$$xp_n(x) = a_{n+1}p_{n+1}(x) + b_np_n(x) + c_np_{n-1}(x) + d_np_{n-2}(x) + \cdots + e_np_0(x). \tag{1.3}$$

Using the orthogonality of the polynomial p_n to the polynomials of lower degree, we have

$$\begin{aligned} d_n\langle p_{n-2}(x), p_{n-2}(x)\rangle_\mu &= \langle xp_n(x), p_{n-2}(x)\rangle_\mu = \int_{\mathbb{R}} xp_n(x)p_{n-2}(x)d\mu \\ &= \langle p_n(x), xp_{n-2}(x)\rangle_\mu = 0. \end{aligned}$$

That is $d_n = 0$. Proceeding in a similar way, we deduce that in the expansion (1.3), only the polynomials p_{n+1}, p_n and p_{n-1} appear:

$$xp_n(x) = a_{n+1}p_{n+1}(x) + b_n p_n(x) + c_n p_{n-1}(x). \tag{1.4}$$

It is not difficult to see that the positivity of μ implies that $a_n c_n > 0$. For the orthonormal polynomials we have the symmetry condition $c_n = a_n$.

The converse of (1.4) is also true and it is the spectral theorem for orthogonal polynomials (it is also known as Favard's theorem [32], although the result seems to be known already to Stieltjes, Chebyshev, and others, and is contained in the book by Stone [81] which appeared a couple of years before Favard's paper).

Theorem 1.2 *If the sequence of polynomials* $(p_n)_n$ *with* $\deg p_n = n$ *satisfies the three-term recurrence relation (1.4) with* $a_n c_n > 0$*, then they are orthogonal with respect to a weight.*

For a proof see [3], [10] or [81].

1.1.3 The classical orthogonal polynomial families

The most important examples of orthogonal polynomials are the so-called classical families. There are three such families (see, for instance, [10, 31, 50, 53, 67, 82], and for a good historical account see [4, 10]).

(1) The Jacobi polynomials $(P_n^{(\alpha,\beta)})_n$, $\alpha, \beta > -1$. They are a double parametric family of orthogonal polynomials with respect to the weight $d\mu = (1-x)^\alpha (1+x)^\beta dx$ on the interval $(-1,1)$. There are some relevant particular values of the parameters which deserve special interest. The simplest case is when $\alpha = \beta = 0$ which results in Legendre polynomials. Legendre introduced them at the end of the 18th century and they are the first example of orthogonal polynomials in history (more about that later). The cases $\alpha = \beta = -1/2$ and $\alpha = \beta = 1/2$ are called Chebyshev polynomials of the first and second kind, respectively, and they were introduced and studied by this Russian mathematician in the second half of the 19th century. When $\alpha = \beta$ we have Gegenbauer or ultraspherical polynomials.

(2) The Laguerre polynomials $(L_n^\alpha)_n$, $\alpha > -1$. They are a single parametric family of orthogonal polynomials with respect to the weight $d\mu(x) = x^\alpha e^{-x} dx$ on the half line $x > 0$.

(3) The Hermite polynomials $(H_n)_n$. They are a single family of orthogonal polynomials with respect to the weight $d\mu(x) = e^{-x^2}dx$ on the real line.

I would like to note that, as usual in mathematics, many of the orthogonal families which appear in these lectures are misnamed, in the sense that someone else introduced them earlier than the person after whom the family is named. The classical families are related to the three most important continuous distribution of probabilities: Beta, Gamma and Normal, respectively. The classical families enjoy a set of important characterization properties that we will discuss in later sections.

There are many other examples of orthogonal polynomials. For instance, the so-called Heine polynomials, a single parametric family of orthogonal polynomials with respect to the weight $d\mu(x) = [x(1-x)(a-x)]^{-1/2}dx$ on the interval $(0,1)$ where $a > 1$ [10]. Of course there are sequences of orthogonal polynomials with no name: as far as I know the orthogonal polynomials with respect to the weight $d\mu(x) = |\cos(x^2+1)|dx$ on the interval $(0,2)$ have not yet been baptized. However, any careful reader will be concerned by the previous examples because actually they are not examples of orthogonal polynomials: they are just examples of weights!

Orthogonal polynomials can be explicitly computed only for a few weights. *Explicitly* means here a closed-form expression for each of the polynomials p_n in the family. For an arbitrary weight (as the one with no name above) one can hardly compute an approximation of the first few orthogonal polynomials. The classical families are among those happy cases in which we can compute *everything* explicitly (most of the identities we will consider next can be found in many books, see, for instance, [10, 31, 50, 53, 67, 82]).

To start with, let us consider the Legendre polynomials $(P_n)_n$, i.e., the Jacobi case with $\alpha = \beta = 0$. They are orthogonal with respect to the Lebesgue measure on the interval $[-1,1]$. Here is a hint for finding explicitly the Legendre polynomials: try with the differentiation formula

$$P_n(x) = ((1-x)^n(1+x)^n)^{(n)}. \tag{1.5}$$

Trivially we get $\deg P_n = n$. We then have to prove that

$$\int_{-1}^{1} P_n(x)x^k dx = 0, \quad 0 \le k \le n-1.$$

This can be easily proved using the following integration by parts:

$$\begin{aligned}
&\int_{-1}^{1}((1-x)^n(1+x)^n)^{(n)}x^k dx \\
&\qquad = ((1-x)^n(1+x)^n)^{(n-1)}x^k\Big|_{-1}^{1} - k\int_{-1}^{1}((1-x)^n(1+x)^n)^{(n-1)}x^{k-1}dx \\
&\qquad = -k\int_{-1}^{1}((1-x)^n(1+x)^n)^{(n-1)}x^{k-1}dx \\
&\qquad = \cdots = (-1)^k k!\int_{-1}^{1}((1-x)^n(1+x)^n)^{(n-k)}dx \\
&\qquad = (-1)^k k!((1-x)^n(1+x)^n)^{(n-1-k)}\Big|_{x=-1}^{x=1} = 0.
\end{aligned}$$

Formula (1.5) is called the Rodrigues' formula for the Legendre polynomials, honoring the French mathematician Olinde Rodrigues who discovered it at the beginning of the 19th century.

Each classical family of orthogonal polynomials has a corresponding Rodrigues' formula of the form

$$p_n(x) = (a_2^n(x)\mu(x))^{(n)}/\mu(x), \tag{1.6}$$

where a_2 is a polynomial of degree at most 2 and μ is the corresponding weight function for the family. More explicitly

(1) Jacobi polynomials

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}((1-x^2)^n(1-x)^\alpha(1+x)^\beta)^{(n)}(1-x)^{-\alpha}(1+x)^{-\beta}.$$

(2) Laguerre polynomials

$$L_n^\alpha(x) = \frac{1}{n!}(x^n x^\alpha e^{-x})^{(n)}e^x x^{-\alpha}.$$

(3) Hermite polynomials

$$H_n(x) = (-1)^n(e^{-x^2})^{(n)}e^{x^2}.$$

One of the characteristic properties of the classical families is precisely this kind of Rodrigues' formula. These Rodrigues' formulas allow an explicit computation for each family. For instance, one get for the Legendre and Laguerre polynomials, respectively

$$\begin{aligned}
P_n(x) &= \frac{1}{2^n}\sum_{k=0}^{[n/2]}(-1)^k\binom{n}{k}\binom{2n-2k}{n}x^{n-2k}, \\
L_n^\alpha(x) &= \sum_{k=0}^{n}\binom{n+\alpha}{n-k}\frac{(-x)^k}{k!}.
\end{aligned} \tag{1.7}$$

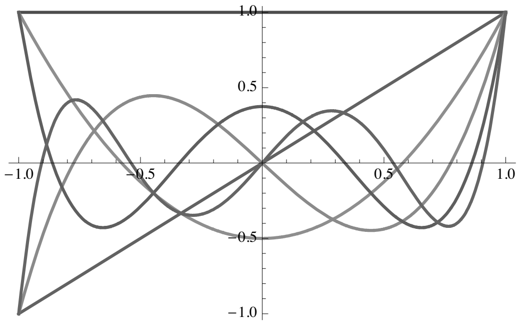

Figure 1.1 The first few Legendre polynomials

Exercise 1.3 Prove the explicit expression for the Laguerre polynomials.

Using the explicit formulas for the Legendre polynomials one can draw the first few of them, as shown in Figure 1.1.

One can then check that each one of these first few Legendre polynomials has real and simple zeros which live in the interval of orthogonality $(-1,1)$. Actually this is a general property of the zeros of orthogonal polynomials.

Theorem 1.4 *The zeros of an orthogonal polynomial p_n with respect to a weight μ are real, simple and live in the convex hull of the support of μ.*

Exercise 1.5 Prove this theorem.
Hint: let $x_1,\dots,x_m$ be the real zeros of p_n with odd multiplicity. Consider then the polynomial $q(x)=(x-x_1)\cdots(x-x_m)$. Show that $p_n(x)q(x)$ has constant sign in $\mathbb{R}$. Use that fact and the orthogonality of p_n to conclude that $m \geq n$.

Rodrigues' formulas can also be used to explicitly compute the three-term recurrence relation (1.4). That is the case for the Hermite polynomials:

$$\begin{aligned} H_{n+1}(x) &= (-1)^{n+1}(e^{-x^2})^{(n+1)}e^{x^2} = (-1)^{n+1}(-2xe^{-x^2})^{(n)}e^{x^2} \\ &= (-1)^{n+1}\left(-2x(e^{-x^2})^{(n)} - 2n(e^{-x^2})^{(n-1)}\right)e^{x^2} \\ &= 2xH_n(x) - 2nH_{n-1}(x). \end{aligned}$$

The three-term recurrence relation for Laguerre and Jacobi polynomials are, respectively

$$L_{n+1}^{\alpha}(x) = \frac{1}{n+1}\left((2n+1+\alpha-x)L_n^{\alpha}(x) - (n+\alpha)L_{n-1}^{\alpha}(x)\right),$$

$$\begin{aligned}2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)P_{n+1}^{(\alpha,\beta)}(x)\\ = -2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)P_{n-1}^{(\alpha,\beta)}(x)\\ +(2n+\alpha+\beta+1)\left[(\alpha^2-\beta^2)\right.\\ \left.+(2n+\alpha+\beta)(2n+\alpha+\beta+2)x\right]P_n^{(\alpha,\beta)}(x).\end{aligned}$$

1.1.4 Second-order differential operator

Legendre polynomials appeared in the context of planetary motion. Indeed, Legendre studied the following potential function related to planetary motion

$$V(t,y,z) = \int\int\int \frac{\rho(u,v,w)}{r}dudvdw,$$

where $r = \sqrt{(t-u)^2+(y-v)^2+(z-w)^2}$, and $\rho(u,v,w)$ stands for the density at the point (u,v,w) (Cartesian coordinates). This integral is easier after performing the change of variable

$$r(\rho,x) = (1-2\rho x+\rho^2)^{1/2}, \quad x = \cos\gamma.$$

Legendre then expanded $1/r(\rho,x)$ in power series of ρ

$$\frac{1}{(1-2\rho x+\rho^2)^{1/2}} = \sum_{n=0}^{\infty}\rho^n P_n(x), \tag{1.8}$$

and he realized that the functions $P_n(x)$ are actually polynomials in x of degree n: they are the polynomials we now call Legendre polynomials.

The function in the left-hand side of identity (1.8) is called the generating function for the Legendre polynomials. The generating function was an invention of the Swiss mathematician Leonard Euler: his genius idea was to pack a sequence $(a_n)_n$ in an analytic function f,

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

so that one can find interesting properties of the sequence $(a_n)_n$ from the function f, as long as one can explicitly find the function f. As the identity (1.8) shows, that is the case of the Legendre polynomials. A very interesting property one can deduce for the Legendre polynomials from its generating function is that they satisfy a second-order differential equation.