APPROXIMATION OF MATRIX FUNCTIONS VIA ORTHOGONAL MATRIX POLYNOMIALS

Manuel Domínguez de la Iglesia¹

Instituto de Matemáticas C.U., UNAM

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Orthogonal Matrix Polynomials

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OUTLINE

1 Orthogonal Polynomials

- Definitions and basic properties
- Differential equations
- Applications

2 Orthogonal Matrix Polynomials

- Definitions and basic properties
- Matrix differential equations
- Applications

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DEFINITIONS AND BASIC PROPERTIES

Let ω be a positive measure on \mathbb{R} and denote $(p_n)_n$ a system of polynomials with deg $p_n = n$ such that they are orthogonal w.r.t. ω , i.e.

$$\int_{\mathbb{R}} p_n(x) p_m(x) d\omega(x) = 0, \quad n \neq m$$

Set $(f,g)_{\omega} = \int_{\mathbb{R}} f(x)g(x)d\omega(x)$ and $||f||_{\omega}^2 = (f,f)_{\omega}$. These are the scalar product and the norm for the weighted function space

$$L^2_{\omega}(\mathbb{R}) = \left\{ f: \mathbb{R} \to \mathbb{R}: \int_{\mathbb{R}} f^2(x) d\omega(x) < \infty
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For any function $f \in L^2_{\omega}(\mathbb{R})$ the series

$$(Sf)(x) = \sum_{k=0}^{\infty} \hat{f}_k \rho_k(x), \quad \hat{f}_k = \frac{(f, \rho_k)_\omega}{\|\rho_k\|_\omega^2}$$

is called the generalized Fourier series of f.

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The series (Sf)(x) converges in average or in the sense of $L^2_{\omega}(\mathbb{R})$, meaning that if $f_n(x) = \sum_{k=0}^n \hat{f}_k p_k(x)$, then the following holds

 $\lim_{n\to\infty}\|f-f_n\|_{\omega}=0$

The polynomial $f_n \in \mathbb{P}_n$ satisfies the following minimization property

$$\|f-f_n\|_{\omega}=\min_{q\in\mathbb{P}_n}\|f-q\|_{\omega}$$

So it is important to compute the coefficients \hat{f}_k . This can be done approximating the integrals using Gaussian quadratures, so the discrete truncation of f is the best approximation of f in the least-squares sense.

Additionally all families of orthogonal polynomials (OPs) $(p_n)_n$ satisfy a three term recurrence relation (Jacobi operator)

$$xp_n(x) = a_n p_{n+1}(x) + b_n p_n(x) + c_n p_{n-1}(x), \quad p_{-1} = 0, \quad p_0 \in \mathbb{R}$$

$$a_n = \frac{(xp_n, p_{n+1})_{\omega}}{(p_{n+1}, p_{n+1})_{\omega}}, \quad b_n = \frac{(xp_n, p_n)_{\omega}}{(p_n, p_n)_{\omega}}, \quad c_n = \frac{(xp_n, p_{n-1})_{\omega}}{(p_{n-1}, p_{n-1})_{\omega}}$$

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DIFFERENTIAL EQUATIONS

Among all families of OPs there are some special instances that have special importance. These families usually satisfy an additional property.

Bochner (1929) (Routh (1884)): characterize $(p_n)_n$ satisfying

 $dp_n \equiv f_2(x)p_n''(x) + f_1(x)p_n'(x) = \lambda_n p_n(x)$

where deg $f_2 \leq 2$ and deg $f_1 = 1$.

This is equivalent to the symmetry (or self-adjointness) of the second-order differential operator

 $d = f_2(x)\partial_x^2 + f_1(x)\partial_x^1$

with respect to $(\cdot, \cdot)_{\omega}$, i.e.

$$(dp_n, p_m)_\omega = (p_n, dp_m)_\omega, \quad n, m \ge 0$$

The relation between the coefficients of the differential operator d and the weight function ω is what is called the Pearson equation

$$(f_2(x)\omega(x))' = f_1(x)\omega(x)$$

plus boundary conditions.

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Orthogonal Matrix Polynomials

CLASSICAL FAMILIES

Hermite:
$$f_2(x) = 1, d\omega(x) = e^{-x^2} dx, x \in \mathbb{R}$$
:
 $H_n(x)'' - 2xH_n(x)' = -2nH_n(x)$
Laguerre: $f_2(x) = x, d\omega(x) = x^{\alpha}e^{-x}dx, \alpha > -1, x \in \mathbb{R}_+$:
 $xL_n^{\alpha}(x)'' + (\alpha + 1 - x)L_n^{\alpha}(x)' = -nL_n^{\alpha}(x)$
Jacobi: $f_2(x) = 1 - x^2, d\omega(x) = (1 - x)^{\alpha}(1 - x)^{\beta}dx, x \in (-1)$
 $(1 - x^2)P_n^{(\alpha,\beta)}(x)'' + (\beta - \alpha - (\alpha + \beta + 2)x)P_n^{(\alpha,\beta)}(x)$
 $-n(n + \alpha + \beta + 1)P_n^{(\alpha,\beta)}(x), \quad \alpha, \beta > -1$

- Chebychev polynomials: when $\alpha = \beta = -1/2$.
- Legendre or spherical polynomials: when $\alpha = \beta = 0$.
- Gegenbauer or ultraspherical polynomials: when $\alpha = \beta = \lambda 1/2$.

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Applications

- Approximation theory: Interpolation, Gaussian integrations, quadrature formulae, least-square approximation, numerical differentiation, etc.
- Operator theory: Jacobi, Hankel or Toeplitz operators.
- Continued fractions.
- Group representation theory: spherical functions.
- Harmonic analysis: Hermite functions are eigenfunctions of the Fourier transform.
- Stochastic processes: Markov chains and diffusion processes.
- Electrostatic equilibrium with logarithmic potential: using zeros of OPs.
- Quantum mechanics: quantum harmonic oscillator, hydrogen atom, etc.

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Matrix-valued polynomials on the real line:

$\boldsymbol{P}(x) = \boldsymbol{C}_n x^n + \boldsymbol{C}_{n-1} x^{n-1} + \dots + \boldsymbol{C}_0, \quad \boldsymbol{C}_i \in \mathbb{C}^{N \times N}, \quad x \in \mathbb{R}$

Krein (1949): orthogonal matrix polynomials (OMP). Orthogonality: weight matrix W (positive definite with finite moments). Let $(P_n)_n$ a system of matrix polynomials with deg P_n and nonsingular leading coefficient such that they are orthogonal in the following sense

$$\langle \boldsymbol{P}_n, \boldsymbol{P}_m \rangle_{\boldsymbol{W}} = \int_{\mathbb{R}} \boldsymbol{P}_n(x) d\boldsymbol{W}(x) \boldsymbol{P}_m^*(x) = \boldsymbol{0}_N, \quad n \neq m$$

This is a *sesquilinear form* and it is not a scalar product in the common sense, but it has properties similar to the usual Hilbert spaces. Now we have the weighted matrix function space

$$L^{2}_{\boldsymbol{W}}(\mathbb{R};\mathbb{C}^{N\times N}) = \left\{ \boldsymbol{F}:\mathbb{R}\to\mathbb{C}^{N\times N}: \int_{\mathbb{R}}\boldsymbol{F}(x)d\boldsymbol{W}(x)\boldsymbol{F}^{*}(x) < \infty \right\}$$

which is a Hilbert space with the norm $\|F\|_W^2 = \mathsf{Tr}(F, \mathsf{F})_{W_{\mathbb{C}}}, \mathbb{C}$

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$$(SF)(x) = \sum_{k=0}^{\infty} \hat{F}_k P_k(x), \quad \hat{F}_k = \langle F, P_k \rangle_W \langle P_k, P_k \rangle_W^{-1}$$

is called the generalized matrix-valued Fourier series of F.

The orthogonality of $(P_n)_n$ with respect to a weight matrix W is equivalent to a three term recurrence relation

$$x P_n(x) = A_n P_{n+1}(x) + B_n P_n(x) + C_n P_{n-1}(x), \quad P_{-1} = 0$$

where A_n and C_n are nonsingular matrices and $B_n = B_n^*$. That means that the OMP are eigenfunctions of a block tridiagonal Jacobi operator:

$$x \begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} B_0 & A_0 \\ C_1 & B_1 & A_1 \\ & C_2 & B_2 & A_2 \\ & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix}$$

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Similarly, for any $\boldsymbol{F} \in L^2_{\boldsymbol{W}}(\mathbb{R}; \mathbb{C}^{N \times N})$, the matrix-valued series

$$(SF)(x) = \sum_{k=0}^{\infty} \hat{F}_k P_k(x), \quad \hat{F}_k = \langle F, P_k \rangle_W \langle P_k, P_k \rangle_W^{-1}$$

is called the generalized matrix-valued Fourier series of F.

The orthogonality of $(\mathbf{P}_n)_n$ with respect to a weight matrix \mathbf{W} is equivalent to a three term recurrence relation

$$x P_n(x) = A_n P_{n+1}(x) + B_n P_n(x) + C_n P_{n-1}(x), \quad P_{-1} = 0$$

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DIFFERENTIAL PROPERTIES

Durán (1997): characterize families of OMP $(P_n)_n$ satisfying

 $\mathcal{D}\boldsymbol{P}_n(x) \equiv \boldsymbol{F}_2(x)\boldsymbol{P}_n'(x) + \boldsymbol{F}_1(x)\boldsymbol{P}_n'(x) + \boldsymbol{F}_0(x)\boldsymbol{P}_n(x) = \boldsymbol{P}_n(x)\Gamma_n$

where $F_2(x)$, $F_1(x)$, $F_0(x)$ are matrix polynomials of degree at most 2, 1 and 0, respectively, and Γ_n is a Hermitian matrix. In this section we will be using the inner product

$$(\boldsymbol{P},\boldsymbol{Q})_{W} = \int_{\mathbb{R}} \boldsymbol{Q}^{*}(x) W(x) \boldsymbol{P}(x) \, dx, \quad (\boldsymbol{P},\boldsymbol{Q})_{W} = \langle \boldsymbol{P}^{*}, \boldsymbol{Q}^{*} \rangle_{W}^{*}$$

The existence of such families is equivalent to the symmetry (or self-adjointness) of the matrix second-order differential operator

$$\mathcal{D} = \boldsymbol{F}_2(x)\partial_x^2 + \boldsymbol{F}_1(x)\partial_x^1 + \boldsymbol{F}_0(x)\partial_x^0$$

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Orthogonal Matrix Polynomials

How to generate examples

- Group Representation Theory: matrix-valued spherical functions associated with different groups (Grünbaum, Pacharoni, Tirao, Román, Zurrián, Koelink).
- Moment equations: from the symmetry equations we solve the corresponding equations (Durán, Grünbaum, MdI). In Durán-MdI (2008) we used this method to generate examples of OMP w.r.t. a weight matrix plus a Dirac delta at one point.
- Matrix-valued bispectral problem: solving the so-called ad-conditions

$$\mathsf{ad}_{oldsymbol{J}}^{k+1}(oldsymbol{\Gamma}) = oldsymbol{0}$$

where k is the order of the differential operator, J is the Jacobi matrix and Γ is a diagonal matrix with the eigenvalues of \mathcal{D} (Castro, Grünbaum, Tirao). It was used to generate examples or order k = 1 in Castro-Grünbaum (2005, 2008).

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• Durán-Grünbaum (2004):

SYMMETRY EQUATIONS (PEARSON EQUATIONS)

$$\begin{aligned} F_2^*(x)W(x) &= W(x)F_2(x) \\ F_1^*(x)W(x) &= (W(x)F_2(x))' - W(x)F_1(x) \\ F_0^*(x)W(x) &= \frac{1}{2}(W(x)F_2(x))'' - (W(x)F_1(x))' + W(x)F_0(x) \end{aligned}$$

$$\lim_{x \to t} \boldsymbol{W}(x) \boldsymbol{F}_2(x) = \boldsymbol{0} = \lim_{x \to t} (\boldsymbol{W}(x) \boldsymbol{F}_1(x) - \boldsymbol{F}_1^*(x) \boldsymbol{W}(x)), \quad t = a, b$$

General method: Suppose $F_2(x) = f_2(x)I$. We factorize $W(x) = \omega(x)T(x)T^*(x)$,

where ω is a classical weight (Hermite, Laguerre o Jacobi) and ${\cal T}$ is a matrix function solution of the first-order differential equation

$$T'(x) = G(x)T(x), \quad T(c) = I, \quad c \in (a, b)$$

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The first symmetry equations is trivial.

Defining

$$\boldsymbol{F}_1(x) = 2f_2(x)\boldsymbol{G}(x) + \frac{(f_2(x)\omega(x))'}{\omega(x)}\boldsymbol{I}$$

the second symmetry equation also holds.

In ally the third symmetry equation is equivalent to

$$(\boldsymbol{W}(x)\boldsymbol{F}_1(x) - \boldsymbol{F}_1^*(x)\boldsymbol{W}(x))' = 2(\boldsymbol{W}(x)\boldsymbol{F}_0 - \boldsymbol{F}_0^*\boldsymbol{W}(x))$$

Therefore, it is enough to find **F**₀ such that

$$\boldsymbol{\chi}(x) = \boldsymbol{T}^{-1}(x) \left(f_2(x) \boldsymbol{G}(x) + f_2(x) \boldsymbol{G}(x)^2 + \frac{(f_2(x)\omega(x))'}{\omega(x)} \boldsymbol{G}(x) - \boldsymbol{F}_0 \right) \boldsymbol{T}(x)$$

is Hermitian for all x.

This method has been generalized when F_2 is not necessarily a scalar function (Durán, 2008).

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EXAMPLES

Let
$$f_2 = I$$
 and $\omega = e^{-x^2}$. Then $G(x) = A + 2Bx$

$$\begin{cases}
\text{Si } B = \mathbf{0} \Rightarrow W(x) = e^{-x^2}e^{Ax}e^{A^*x} \\
\text{Si } A = \mathbf{0} \Rightarrow W(x) = e^{-x^2}e^{Bx^2}e^{B^*x^2}
\end{cases}$$

In the first case, a possible solution for the matrix function

$$\boldsymbol{\chi}(\boldsymbol{x}) = \boldsymbol{A}^2 - 2\boldsymbol{A}\boldsymbol{x} - e^{-\boldsymbol{A}\boldsymbol{x}}\boldsymbol{F}_0 e^{\boldsymbol{A}\boldsymbol{x}}$$

to be Hermitian is choosing $\boldsymbol{F}_0 = \boldsymbol{A}^2 - 2\boldsymbol{J}$, where

$$\boldsymbol{A} = \begin{pmatrix} 0 & \nu_1 & 0 & \cdots & 0 \\ 0 & 0 & \nu_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \nu_{N-1} \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad \boldsymbol{J} = \begin{pmatrix} N-1 & 0 & \cdots & 0 & 0 \\ 0 & N-2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

In the second case, a possible solution for the matrix function

$$\chi(x) = 2\mathbf{B} + (4\mathbf{B}^2 - 4\mathbf{B})x^2 - e^{-\mathbf{B}x^2}\mathbf{F}_0e^{\mathbf{B}x^2}$$

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EXAMPLES

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$$G(x) = \mathbf{A} + \frac{\mathbf{B}}{x}$$

$$\begin{cases} \text{If } \mathbf{B} = \mathbf{0} \Rightarrow x^{\alpha} e^{-x} e^{\mathbf{A}x} e^{\mathbf{A}^* x} \\ \text{If } \mathbf{A} = \mathbf{0} \Rightarrow x^{\alpha} e^{-x} x^{\mathbf{B}} x^{\mathbf{B}} \end{cases}$$

and for $f_2 = (1 - x^2)I$ and $\omega = (1 - x)^{\alpha}(1 + x)^{\beta}$. Then

$$\boldsymbol{G}(x) = \frac{\boldsymbol{A}}{1-x} + \frac{\boldsymbol{B}}{1+x}$$

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Examples have also been found where the matrices **A** and **B** do not commute (Durán-MdI and Grünbaum-Pacharoni-Tirao), and a second seco

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NEW PHENOMENA

- For a fixed family of OMP, there may exist several linear independent matrix differential operators having the family of OMP as eigenfunctions (Castro, Durán, Mdl, Grünbaum, Pacharoni, Tirao, Román).
- For a fixed matrix differential operator, there may exist infinite linear independent families of OMP that are eigenfunctions of the same fixed differential operator (Durán, MdI).
- There exist examples of OMP satisfying odd-order matrix differential equations (Castro, Grünbaum, Durán, MdI).
- There exist families of ladder operators (annihilation and creation or lowering and raising) for some examples of OMP, some of them of 0-th order (Grünbaum, MdI, Martínez-Finkelshtein).

Applications

 Gaussian quadrature formulae: for any F, G ∈ L²_W(ℝ; C^{N×N}) it is possible to approximate the integral

$$\int_{\mathbb{R}} \boldsymbol{F}(x) d\boldsymbol{W}(x) \boldsymbol{G}^{*}(x) \approx \sum_{k=1}^{m} \boldsymbol{F}(x_{k}) \Lambda_{k} \boldsymbol{G}^{*}(x_{k})$$

where x_k are the zeros of the OMP P_k (i.e. det $P_k(x) = 0$) counting all multiplicities and Λ_k are certain matrices (van Assche-Sinap, Durán-Polo).

• Sobolev orthogonal polynomials: It has been found a relation between Sobolev OPs with the inner product

$$\langle p_n, p_m \rangle = \int p_n p_m d\mu + \sum_{i=1}^M \sum_{j=0}^{M_i} \lambda_{ij} p_n^{(j)}(c_i) p_m^{(j)}(c_i) = \delta_{nm}, \quad c_i \in \mathbb{R}$$

and OMP. The reason is that the Sobolev OPs satisfy certain higher-order difference equation, so it is possible to rewrite them in terms of OMP (Durán-van Assche).

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Applications

• Bivariate Markov processes: The block tridiagonal structure of the Jacobi matrix for OMP is suitable for some processes called *quasi-birth-and-death processes*, defined on two-dimensional grids (Grünbaum, Dette, Reuther, Zygmunt, Clayton).

Additionally, the examples of OMP satisfying second-order differential equations are suitable for some processes called *switching diffusion processes*. Here we have a collection of N phases where a different diffusion is performed in each phase and is jumping to other phases according to a continuous time Markov chain (MdI).

 Other applications: scattering theory (Geronimo), Lanczos method for block matrices (Golub, Underwood), time-and-band limiting problems (Durán, Grünbaum, Pacharoni, Zurrián), noncommutative integrable systems and Painlevé equations (Cafasso, MdI), etc.

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