Approximation of matrix functions via 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
Orthogonal Polynomials

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   - Definitions and basic properties
   - Differential equations
   - Applications

2. Orthogonal Matrix Polynomials
   - Definitions and basic properties
   - Matrix differential equations
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Orthogonal Polynomials

DEFINITIONS AND BASIC PROPERTIES

Let $\omega$ 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. $\omega$, 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

$$L^2_\omega(\mathbb{R}) = \left\{ f : \mathbb{R} \to \mathbb{R} : \int_{\mathbb{R}} f^2(x)d\omega(x) < \infty \right\}$$

For any function $f \in L^2_\omega(\mathbb{R})$ the series

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

is called the generalized Fourier series of $f$. 

Orthogonal Matrix Polynomials
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Definitions and Basic Properties

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)
\[
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, \quad p_0 \in \mathbb{R}
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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

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dp_n = f_2(x)p''_n(x) + f_1(x)p'_n(x) = \lambda np_n(x)
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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

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d = f_2(x)\partial_x^2 + f_1(x)\partial_x^1
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with respect to \((\cdot, \cdot)_\omega\), i.e.

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(dp_n, p_m)_\omega = (p_n, dp_m)_\omega, \quad n, m \geq 0
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The relation between the coefficients of the differential operator \(d\) and the weight function \(\omega\) is what is called the Pearson equation

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**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)
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**Laguerre:** \( f_2(x) = x, \ d\omega(x) = x^\alpha e^{-x} \, dx, \ \alpha > -1, \ x \in \mathbb{R}_+: \)

\[
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**Jacobi:** \( f_2(x) = 1 - x^2, \ d\omega(x) = (1 - x)^\alpha (1 - x)^\beta \, dx, \ x \in (-1, 1): \)

\[
(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), \ \alpha, \beta > -1
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Among the Jacobi polynomials we have the well known

- **Chebychev polynomials:** when \( \alpha = \beta = -1/2. \)
- **Legendre or spherical polynomials:** when \( \alpha = \beta = 0. \)
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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.
- ...
Outline

1. **Orthogonal Polynomials**
   - Definitions and basic properties
   - Differential equations
   - Applications

2. **Orthogonal Matrix Polynomials**
   - Definitions and basic properties
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**Definitions and Basic Properties**

Matrix-valued polynomials on the real line:

$$P(x) = C_n x^n + C_{n-1} x^{n-1} + \cdots + C_0, \quad C_i \in \mathbb{C}^{N \times N}, \quad x \in \mathbb{R}$$

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

$$\langle P_n, P_m \rangle_W = \int_{\mathbb{R}} P_n(x) dW(x) P_m^*(x) = 0_N, \quad n \neq m$$

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

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

which is a Hilbert space with the norm $\|F\|_W^2 = \text{Tr}(F \cdot F^\ast)_W$. 
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**Definitions and Basic Properties**

Similarly, for any $F \in L^2_W(\mathbb{R}; \mathbb{C}^{N \times N})$, 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 $(P_n)_n$ with respect to a weight matrix $W$ is equivalent to a three term recurrence relation

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

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:

$$x \begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} B_0 & A_0 \\ C_1 & B_1 & A_1 \\ C_2 & B_2 & A_2 \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} P_0(x) \\ P_1(x) \\ P_2(x) \\ \vdots \end{pmatrix}$$
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The orthogonality of $(P_n)_n$ with respect to a weight matrix $W$ is equivalent to a three term recurrence relation

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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:

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

Similarly, for any $F \in L^2_W(\mathbb{R}; \mathbb{C}^{N \times N})$, 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 $F$.*

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

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

\[
\mathcal{D}P_n(x) \equiv F_2(x)P_n''(x) + F_1(x)P_n'(x) + F_0(x)P_n(x) = P_n(x)\Gamma_n
\]

where \(F_2(x), F_1(x), F_0(x)\) are matrix polynomials of degree at most 2, 1 and 0, respectively, and \(\Gamma_n\) is a Hermitian matrix.

In this section we will be using the inner product

\[
(P, Q)_W = \int_{\mathbb{R}} Q^*(x)W(x)P(x)\,dx, \quad (P, Q)_W = \langle P^*, Q^* \rangle_W^*
\]

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

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\mathcal{D} = F_2(x)\partial_x^2 + F_1(x)\partial_x^1 + F_0(x)\partial_x^0
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with \(\mathcal{D}P_n = P_n\Gamma_n\)

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How to generate examples

- **Group Representation Theory**: matrix-valued spherical functions associated with different groups (Gr"unbaum, Pacharoni, Tirao, Román, Zurrián, Koelink).

- Moment equations: from the symmetry equations we solve the corresponding equations (Durán, Gr"unbaum, 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

\[
\text{ad}_{J}^{k+1}(\Gamma) = 0
\]

where \( k \) is the order of the differential operator, \( J \) is the Jacobi matrix and \( \Gamma \) is a diagonal matrix with the eigenvalues of \( D \) (Castro, Gr"unbaum, Tirao). It was used to generate examples or order \( k = 1 \) in Castro-Gr"unbaum (2005, 2008).
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**Symmetry Equations (Pearson Equations)**

\[
F^*_2(x)W(x) = W(x)F_2(x) \\
F^*_1(x)W(x) = (W(x)F_2(x))' - W(x)F_1(x) \\
F^*_0(x)W(x) = \frac{1}{2}(W(x)F_2(x))'' - (W(x)F_1(x))' + W(x)F_0(x)
\]

\[
\lim_{x \to t} W(x)F_2(x) = 0 = \lim_{x \to t} (W(x)F_1(x) - F^*_1(x)W(x)), \quad t = a, b
\]

General method: Suppose \(F_2(x) = f_2(x)I\). We factorize

\[
W(x) = \omega(x)T(x)T^*(x),
\]

where \(\omega\) is a classical weight (Hermite, Laguerre or Jacobi) and \(T\) is a matrix function solution of the first-order differential equation

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T'(x) = G(x)T(x), \quad T(c) = I, \quad c \in (a, b)
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The first symmetry equation is trivial.

Defining

$$F_1(x) = 2f_2(x)G(x) + \frac{(f_2(x)\omega(x))'}{\omega(x)} I$$

the second symmetry equation also holds.

Finally the third symmetry equation is equivalent to

$$(W(x)F_1(x) - F_1^*(x)W(x))' = 2(W(x)F_0 - F_0^*W(x))$$

Therefore, it is enough to find $F_0$ such that

$$\chi(x) = T^{-1}(x)\left(f_2(x)G(x) + f_2(x)G(x)^2 + \frac{(f_2(x)\omega(x))'}{\omega(x)} G(x) - F_0\right) T(x)$$

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 \( G(x) = A + 2Bx \)

\[
\begin{align*}
\text{Si } B = 0 & \Rightarrow W(x) = e^{-x^2} e^{Ax} e^{A^*x} \\
\text{Si } A = 0 & \Rightarrow W(x) = e^{-x^2} e^{Bx^2} e^{B^*x^2}
\end{align*}
\]

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

\[
\chi(x) = A^2 - 2Ax - e^{-Ax} F_0 e^{Ax}
\]

to be Hermitian is choosing \( F_0 = A^2 - 2J \), where

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

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

\[
\chi(x) = 2B + (4B^2 - 4B)x^2 - e^{-Bx^2} F_0 e^{Bx^2}
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The same can be done for $f_2 = xI$ and $\omega = x^\alpha e^{-x}$. Then

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

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

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

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

$$\begin{cases} 
    \text{If } B = 0 \Rightarrow (1 - x)^\alpha (1 + x)^\beta (1 - x)^A (1 - x)^A \\
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Examples have also been found where the matrices $A$ and $B$ do not commute (Durán-MdI and Grünbaum-Pacharoni-Tirao).
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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, MdI, 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).
Orthogonal Polynomials

**Applications**

- **Gaussian quadrature formulae:** for any $F, G \in L^2_W(\mathbb{R}; \mathbb{C}^{N \times N})$ it is possible to approximate the integral

$$\int_{\mathbb{R}} F(x) dW(x) G^*(x) \approx \sum_{k=1}^{m} F(x_k) \Lambda_k G^*(x_k)$$

where $x_k$ are the zeros of the OMP $P_k$ (i.e. $\det P_k(x) = 0$) counting all multiplicities and $\Lambda_k$ 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 (Grüenbaum, 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, Grüenbaum, Pacharoni, Zurrián), noncommutative integrable systems and Painlevé equations (Cafasso, MdI), etc.
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