# 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
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## Definitions and basic properties

Let $\omega$ be a positive measure on $\mathbb{R}$ and denote $\left(p_{n}\right)_{n}$ a system of polynomials with $\operatorname{deg} p_{n}=n$ 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


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


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L_{\omega}^{2}(\mathbb{R})=\left\{f: \mathbb{R} \rightarrow \mathbb{R}: \int_{\mathbb{R}} f^{2}(x) d \omega(x)<\infty\right\}
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$$
(S f)(x)=\sum_{k=0}^{\infty} \hat{f}_{k} p_{k}(x), \quad \hat{f}_{k}=\frac{\left(f, p_{k}\right)_{\omega}}{\left\|p_{k}\right\|_{\omega}^{2}}
$$

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## Definitions and basic properties

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

$$
\lim _{n \rightarrow \infty}\left\|f-f_{n}\right\|_{\omega}=0
$$

The polynomial $f_{n} \in \mathbb{P}_{n}$ satisfies the following minimization property

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) $\left(p_{n}\right)_{n}$ satisfy a three term recurrence relation (Jacobi operator)

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$$
x p_{n}(x)=a_{n} p_{n+1}(x)+b_{n} p_{n}(x)+c_{n} p_{n-1}(x), \quad p_{-1}=0, \quad p_{0} \in \mathbb{R}
$$

where

$$
a_{n}=\frac{\left(x p_{n}, p_{n+1}\right)_{\omega}}{\left(p_{n+1}, p_{n+1}\right)_{\omega}}, \quad b_{n}=\frac{\left(x p_{n}, p_{n}\right)_{\omega}}{\left(p_{n}, p_{n}\right)_{\omega}}, \quad c_{n}=\frac{\left(x p_{n}, p_{n-1}\right)_{\omega}}{\left(p_{n-1}, p_{n-1}\right)_{\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 ( $\left.p_{n}\right)_{n}$ satisfying $d p_{n} \equiv f_{2}(x) p_{n}^{\prime \prime}(x)+f_{1}(x) p_{n}^{\prime}(x)=\lambda_{n} p_{n}(x)$
where $\operatorname{deg} f_{2} \leq 2$ and $\operatorname{deg} f_{1}=1$
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 $(\cdot, \cdot)_{\omega}, i . e$.
$\left(d p_{n}, p_{m}\right)_{\omega}=\left(p_{n}, d p_{m}\right)_{\omega}, \quad n, m \geq 0$
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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\left(f_{2}(x) \omega(x)\right)^{\prime}=f_{1}(x) \omega(x)
$$

plus boundary conditions.

## Classical families

Hermite: $f_{2}(x)=1, d \omega(x)=\mathrm{e}^{-x^{2}} d x, x \in \mathbb{R}$ :

$$
H_{n}(x)^{\prime \prime}-2 x H_{n}(x)^{\prime}=-2 n H_{n}(x)
$$

Laguerre: $f_{2}(x)=x, d \omega(x)=x^{\alpha} e^{-x} d x, \alpha>-1, x \in \mathbb{R}_{+}$

$$
x L_{n}^{\alpha}(x)^{\prime \prime}+(\alpha+1-x) L_{n}^{\alpha}(x)^{\prime}=-n L_{n}^{\alpha}(x)
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Jacobi: $f_{2}(x)=1-x^{2}, d \omega(x)=(1-x)^{\alpha}(1-x)^{\beta} d x, x \in(-1,1)$ :


Among the Jacobi polynomials we have the well known

- 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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$J$ Jacobi: $f_{2}(x)=1-x^{2}, d \omega(x)=(1-x)^{\alpha}(1-x)^{\beta} d x, x \in(-1,1)$ :
 $-n(n+\alpha+\beta+1) P_{n}^{(\alpha, \beta)}(x), \quad \alpha, \beta>-1$
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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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## Definitions and basic properties

Matrix-valued polynomials on the real line:

$$
\boldsymbol{P}(x)=\boldsymbol{C}_{n} x^{n}+\boldsymbol{C}_{n-1} x^{n-1}+\cdots+\boldsymbol{C}_{0}, \quad \boldsymbol{C}_{i} \in \mathbb{C}^{N \times N}, \quad x \in \mathbb{R}
$$

Krein (1949): orthogonal matrix polynomials (OMP)
Orthogonality: weight matrix $\boldsymbol{W}$ (positive definite with finite moments).
Let $\left(\boldsymbol{P}_{n}\right)_{n}$ a system of matrix polynomials with $\operatorname{deg} \boldsymbol{P}_{n}$ and nonsingular leading coefficient such that they are orthogonal in the following sense

$$
\left\langle\boldsymbol{P}_{n}, \boldsymbol{P}_{m}\right\rangle \boldsymbol{w}=\int_{\mathbb{R}} \boldsymbol{P}_{n}(x) d \boldsymbol{W}(x) \boldsymbol{P}_{m}^{*}(x)=\mathbf{0}_{N}, \quad n \neq m
$$

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_{W}^{2}\left(\mathbb{R} ; \mathbb{C}^{N \times N}\right)=\left\{\boldsymbol{F}: \mathbb{R} \rightarrow \mathbb{C}^{N \times N}: \int_{\mathbb{R}} \boldsymbol{F}(x) d \boldsymbol{W}(x) \boldsymbol{F}^{*}(x)<\infty\right\}
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which is a Hilbert space with the norm $\|\boldsymbol{F}\|_{w}^{2}=\operatorname{Tr}\langle\boldsymbol{F}, \boldsymbol{F}\rangle \boldsymbol{w}$.

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(S \boldsymbol{F})(x)=\sum_{k=0}^{\infty} \hat{\boldsymbol{F}}_{k} \boldsymbol{P}_{k}(x), \quad \hat{\boldsymbol{F}}_{k}=\left\langle\boldsymbol{F}, \boldsymbol{P}_{k}\right\rangle \boldsymbol{w}\left\langle\boldsymbol{P}_{k}, \boldsymbol{P}_{k}\right\rangle_{\boldsymbol{w}}^{-1}
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is called the generalized matrix-valued Fourier series of $\boldsymbol{F}$.
The orthogonality of $\left(P_{n}\right)_{n}$ with respect to a weight matrix $W$ is equivalent to a three term recurrence relation
where $\boldsymbol{A}_{n}$ and $\boldsymbol{C}_{n}$ are nonsingular matrices and $\boldsymbol{B}_{n}=\boldsymbol{B}_{n}^{*}$
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$$
x\left(\begin{array}{c}
\boldsymbol{P}_{0}(x) \\
\boldsymbol{P}_{1}(x) \\
\boldsymbol{P}_{2}(x) \\
\vdots
\end{array}\right)=\left(\begin{array}{ccccc}
\boldsymbol{B}_{0} & \boldsymbol{A}_{0} & & & \\
\boldsymbol{C}_{1} & \boldsymbol{B}_{1} & \boldsymbol{A}_{1} & & \\
& \boldsymbol{C}_{2} & \boldsymbol{B}_{2} & \boldsymbol{A}_{2} & \\
& & \ddots & \ddots & \ddots
\end{array}\right)\left(\begin{array}{c}
\boldsymbol{P}_{0}(x) \\
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\boldsymbol{P}_{2}(x) \\
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\end{array}\right)
$$

## Differential properties

Durán (1997): characterize families of OMP $\left(\boldsymbol{P}_{n}\right)_{n}$ satisfying

$$
\mathcal{D} \boldsymbol{P}_{n}(x) \equiv \boldsymbol{F}_{2}(x) \boldsymbol{P}_{n}^{\prime \prime}(x)+\boldsymbol{F}_{1}(x) \boldsymbol{P}_{n}^{\prime}(x)+\boldsymbol{F}_{0}(x) \boldsymbol{P}_{n}(x)=\boldsymbol{P}_{n}(x) \boldsymbol{\Gamma}_{n}
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where $\boldsymbol{F}_{2}(x), \boldsymbol{F}_{1}(x), \boldsymbol{F}_{0}(x)$ are matrix polynomials of degree at most 2,1 and 0 , respectively, and $\boldsymbol{\Gamma}_{n}$ is a Hermitian matrix.

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$$
(\boldsymbol{P}, \boldsymbol{Q})_{\boldsymbol{w}}=\int_{\mathbb{R}} \boldsymbol{Q}^{*}(x) \boldsymbol{W}(x) \boldsymbol{P}(x) d x, \quad(\boldsymbol{P}, \boldsymbol{Q})_{\boldsymbol{w}}=\left\langle\boldsymbol{P}^{*}, \boldsymbol{Q}^{*}\right\rangle_{\boldsymbol{w}}^{*}
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Durán (1997): characterize families of $\operatorname{OMP}\left(\boldsymbol{P}_{n}\right)_{n}$ satisfying

$$
\mathcal{D} \boldsymbol{P}_{n}(x) \equiv \boldsymbol{F}_{2}(x) \boldsymbol{P}_{n}^{\prime \prime}(x)+\boldsymbol{F}_{1}(x) \boldsymbol{P}_{n}^{\prime}(x)+\boldsymbol{F}_{0}(x) \boldsymbol{P}_{n}(x)=\boldsymbol{P}_{n}(x) \boldsymbol{\Gamma}_{n}
$$

where $\boldsymbol{F}_{2}(x), \boldsymbol{F}_{1}(x), \boldsymbol{F}_{0}(x)$ are matrix polynomials of degree at most 2,1 and 0 , respectively, and $\boldsymbol{\Gamma}_{n}$ is a Hermitian matrix. In this section we will be using the inner product

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

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

$$
\begin{aligned}
& \mathcal{D}=\boldsymbol{F}_{2}(x) \partial_{x}^{2}+\boldsymbol{F}_{1}(x) \partial_{x}^{1}+\boldsymbol{F}_{0}(x) \partial_{x}^{0} \\
& \text { with } \quad \mathcal{D} \boldsymbol{P}_{n}=\boldsymbol{P}_{n} \boldsymbol{\Gamma}_{n}
\end{aligned}
$$

$\mathcal{D}$ is symmetric w.r.t. $\boldsymbol{W}$ if $(\mathcal{D} \boldsymbol{P}, \boldsymbol{Q})_{w}=(\boldsymbol{P}, \mathcal{D} \boldsymbol{Q})_{w}$

## 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

where $k$ is the order of the differential operator, $J$ is the Jacobi matrix and $\boldsymbol{\Gamma}$ 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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\operatorname{ad}_{J}^{k+1}(\boldsymbol{\Gamma})=\mathbf{0}
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- Durán-Grünbaum (2004):


## Symmetry equations (Pearson equations)

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\begin{aligned}
& \boldsymbol{F}_{2}^{*}(x) \boldsymbol{W}(x)=\boldsymbol{W}(x) \boldsymbol{F}_{2}(x) \\
& \boldsymbol{F}_{1}^{*}(x) \boldsymbol{W}(x)=\left(\boldsymbol{W}(x) \boldsymbol{F}_{2}(x)\right)^{\prime}-\boldsymbol{W}(x) \boldsymbol{F}_{1}(x) \\
& \boldsymbol{F}_{0}^{*}(x) \boldsymbol{W}(x)=\frac{1}{2}\left(\boldsymbol{W}(x) \boldsymbol{F}_{2}(x)\right)^{\prime \prime}-\left(\boldsymbol{W}(x) \boldsymbol{F}_{1}(x)\right)^{\prime}+\boldsymbol{W}(x) \boldsymbol{F}_{0}(x)
\end{aligned}
$$

$$
\lim _{x \rightarrow t} \boldsymbol{W}(x) \boldsymbol{F}_{2}(x)=\mathbf{0}=\lim _{x \rightarrow t}\left(\boldsymbol{W}(x) \boldsymbol{F}_{1}(x)-\boldsymbol{F}_{1}^{*}(x) \boldsymbol{W}(x)\right), \quad t=a, b
$$

## General method: Suppose $\boldsymbol{F}_{2}(x)=f_{2}(x) \boldsymbol{I}$. We factorize

$$
\boldsymbol{W}(x)=\omega(x) \boldsymbol{T}(x) \boldsymbol{T}^{*}(x)
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where $\omega$ is a classical weight (Hermite, Laguerre o Jacobi) and $T$ is a matrix function solution of the first-order differential equation


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$$
\boldsymbol{T}^{\prime}(x)=\boldsymbol{G}(x) \boldsymbol{T}(x), \quad \boldsymbol{T}(c)=\boldsymbol{I}, \quad c \in(a, b)
$$

(1) The first symmetry equations is trivial.
(3) Defining

$$
\boldsymbol{F}_{1}(x)=2 f_{2}(x) \boldsymbol{G}(x)+\frac{\left(f_{2}(x) \omega(x)\right)^{\prime}}{\omega(x)} \boldsymbol{I}
$$

the second symmetry equation also holds.
a Finally the third symmetry equation is equivalent to

$$
\left(\boldsymbol{W}(x) \boldsymbol{F}_{1}(x)-\boldsymbol{F}_{1}^{*}(x) \boldsymbol{W}(x)\right)^{\prime}=2\left(\boldsymbol{W}(x) \boldsymbol{F}_{0}-\boldsymbol{F}_{0}^{*} \boldsymbol{W}(x)\right)
$$

Therefore, it is enough to find $\boldsymbol{F}_{0}$ such that
$x(x)=T^{-1}(x)\left(f_{2}(x) G(x)+f_{2}(x) G(x)^{2}+\frac{\left(f_{2}(x) \omega(x)\right)^{\prime}}{\omega(x)} G(x)-F_{0}\right) T(x)$
is Hermitian for all $x$.

This method has been generalized when $\boldsymbol{F}_{2}$ is not necessarily a scalar function (Durán, 2008).
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## EXAMPLES

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

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\text { Si } \boldsymbol{B}=\mathbf{0} \Rightarrow \boldsymbol{W}(x)=e^{-x^{2}} e^{\boldsymbol{A} x} e^{\boldsymbol{A}^{*} x} \\
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\end{array}\right.
$$

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

$$
\chi(x)=\boldsymbol{A}^{2}-2 \boldsymbol{A} x-e^{-\boldsymbol{A} x} \boldsymbol{F}_{0} e^{\boldsymbol{A} x}
$$

to be Hermitian is choosing $\boldsymbol{F}_{0}=\boldsymbol{A}^{2}-2 \boldsymbol{J}$, where


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

$$
\chi^{\prime}(x)=2 \boldsymbol{B}+\left(4 \boldsymbol{B}^{2}-4 \boldsymbol{B}\right) x^{2}-e^{-\boldsymbol{B} x^{2}} \boldsymbol{F}_{0} e^{\boldsymbol{B} x^{2}}
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$\boldsymbol{A}=\left(\begin{array}{ccccc}0 & \nu_{1} & 0 & \cdots & 0 \\ 0 & 0 & \nu_{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \nu_{N-1} \\ 0 & 0 & 0 & \cdots & 0\end{array}\right), \quad \boldsymbol{J}=\left(\begin{array}{ccccc}N-1 & 0 & \cdots & 0 & 0 \\ 0 & N-2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0\end{array}\right)$
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\end{array}\right), \quad \boldsymbol{J}=\left(\begin{array}{ccccc}
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## EXAMPLES

The same can be done for $f_{2}=x I$ and $\omega=x^{\alpha} e^{-x}$. Then

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\boldsymbol{G}(x)=\boldsymbol{A}+\frac{\boldsymbol{B}}{x} \\
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\end{array}\right.
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and for $f_{2}=\left(1-x^{2}\right)$ I and $\omega=(1-x)^{\alpha}(1+x)^{\beta}$. Then


Examples have also been found where the matrices $\boldsymbol{A}$ and $B$ do


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Examples have also been found where the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ do not commute (Durán-MdI and Grünbaum-Pacharoni-Tirao).

## 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 $\boldsymbol{F}, \boldsymbol{G} \in L_{W}^{2}\left(\mathbb{R} ; \mathbb{C}^{N \times N}\right)$ it is possible to approximate the integral

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

where $x_{k}$ are the zeros of the OMP $\boldsymbol{P}_{k}$ (i.e. $\operatorname{det} \boldsymbol{P}_{k}(x)=0$ ) counting all multiplicities and $\boldsymbol{\Lambda}_{k}$ are certain matrices (van Assche-Sinap, Durán-Polo).
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- Sobolev orthogonal polynomials: It has been found a relation between Sobolev OPs with the inner product

$$
\left\langle p_{n}, p_{m}\right\rangle=\int p_{n} p_{m} d \mu+\sum_{i=1}^{M} \sum_{j=0}^{M_{i}} \lambda_{i j} p_{n}^{(j)}\left(c_{i}\right) p_{m}^{(j)}\left(c_{i}\right)=\delta_{n m}, \quad c_{i} \in \mathbb{R}
$$

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).

## 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).



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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 (Mdl).
- 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.

