Orthogonal functions and matrix computations

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Introduction

Many results involving orthogonal functions can be translated into matrix language and vice versa.

Two examples:

- recurrence relations
- spectral transformations

Example 1: three-term recurrence relation

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Consider inner product on the real line

$$\langle p, q \rangle = \int_{\mathbb{R}} p(x)q(x)d\mu(x).$$

Orthogonal polynomials p_i satisfy a three-term recurrence relation

$$xp_n(x) = a_n p_{n+1}(x) + b_n p_n(x) + a_{n-1}p_{n-1}(x).$$

In matrix language

$$x\,[p_0(x), p_1(x), p_2(x), \ldots] = [p_0(x), p_1(x), p_2(x), \ldots]\,J$$

with J the Jacobi matrix

$$J = \begin{bmatrix} b_0 & a_0 & & \\ a_0 & b_1 & a_1 & \\ & a_1 & b_2 & \ddots \\ & & \ddots & \ddots \end{bmatrix}.$$

Example 2: spectral transformation

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Two related inner products $\langle\cdot\rangle_\mu$ and $\langle\cdot\rangle_\nu$

$$\langle p, q \rangle_\mu = \int_{\mathbb{R}} p(x)q(x)d\mu(x)$$
$$\langle p, q \rangle_\nu = \int_{\mathbb{R}} p(x)q(x)\mathbf{d\nu(x)} = \int_{\mathbb{R}} p(x)q(x)\mathbf{(x-\beta)d\mu(x)}$$

Relation between Jacobi matrices J_μ and J_ν associated with μ and ν, respectively:

$$J_\mu - \beta I = L\,L^T$$
$$J_\nu - \beta I = L^T L$$

- Agrees with one step of a semi-infinite Cholesky LR algorithm
- L is lower bidiagonal

[Bueno, Marcellán, Dopico]
[Galant], [Kautsky, Golub], [Watkins], ...

Discrete inner product

Given the basis functions $p_1(z), p_2(z), \ldots$,
n points $z_i \in \mathbb{C}$ and corresponding weights $w_i > 0$,
define within the vector space $\mathcal{P}^n = \{\sum_{i=1}^n c_i p_i(z)\}$ the discrete inner product:

$$\langle p, q \rangle = \sum_{i=1}^{n} w_i^2 \overline{p(z_i)} q(z_i). \tag{1}$$

Let $\{a_j(z)\}$ be the orthonormal functions, i.e., $\langle a_i, a_j \rangle = \delta_{ij}$, such that $a_j(z) \in \mathcal{P}^j \setminus \mathcal{P}^{j-1}$, $j = 1, 2, \ldots, n$.

Discrete LS approximation with orthonormal functions

Given: a function $f(z)$
Find: the function $p(z) = \sum_{i=1}^{\alpha} c_i p_i(z)$ with $\alpha \leq n$ s.t.

$$\sum_{i=1}^{n} w_i^2 |f(z_i) - p(z_i)|^2 \quad \text{is minimal.}$$

Solution: The solution $p(z)$ can be represented as
$p(z) = \sum_{j=1}^{\alpha} c_j a_j(z)$ with $c_j = \langle a_j, f \rangle$.
Thus LS problem is reduced to the problem of computing $a_j(z)$.

Computing the recurrence parameters

For many important choices of the basis functions $p_i(z)$ of the vector space $\mathcal{P}^n = \{\sum_{i=1}^n c_i p_i(z)\}$, computing the recurrence parameters for the corresponding orthonormal functions $a_i(z)$ reduces to an inverse eigenvalue problem (IEP). Choices for the basis functions $p_i(z)$:

- $1, z, z^2, z^3, \ldots$ (orthogonal polynomials, OP)
- $1, z, z^{-1}, z^2, z^{-2}, z^3, z^{-3}, \ldots$ (orthogonal Laurent polynomials)
- any sequence such that z^k with $k > 0$ comes after z^{k-1} and z^{-k} with $k > 0$ comes after $z^{-(k-1)}$ (general orthogonal Laurent polynomials)
- $1, \frac{1}{z-y_1}, \frac{1}{z-y_2}, \ldots$ (orthogonal proper rational functions)
- ...

This can be extended to:

- multivariate orthogonal functions
- vector and matrix cases
- ...

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General Scheme

Given: the nodes z_i and the corresponding weights w_i, $i = 1, 2, \ldots, n$ of the discrete inner product.
Based on the nodes, one or more $n \times n$ diagonal matrices are derived: $D_1, D_2, \ldots$.

Definition (general IEP)

Given: $D_1, D_2, \ldots$ – diagonal matrices, $\mathbf{w} = (w_i)$ – weights
Find: Unitary matrix Q and matrices H_j having a specific structure such that

$$Q^H \mathbf{w} = \|\mathbf{w}\| \mathbf{e}_1, \quad Q^H D_j Q = H_j.$$

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Comments

- The structure of the matrix(ces) H_j is determined by the recurrence relation for the orthonormal functions $a_i(z)$.
- The columns of the unitary matrix Q_i are connected to the orthonormal functions as follows:

$$Q_k = diag(w_i)[a_k(z_i)]_{i=1,2,\ldots,n}.$$

- The columns Q_k satisfy a corresponding recurrence relation.
- The orthonormality of the functions $a_k(z)$ is equivalent to Q being unitary:

$$\begin{aligned}\langle a_j(z), a_k(z) \rangle &= \sum_{i=1}^{n} w_i^2 \overline{a_j(z_i)} a_k(z_i) \\ &= Q_j^H Q_k \\ &= \delta_{jk}\end{aligned}$$

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Illustrations

In this talk:

- orthonormal polynomials in one variable
  [Reichel, Ammar, Gragg][Elhay, Golub, Kautsky][Golub, Meurant]
- orthonormal polynomials in two variables
  [VB, Chesnokov]
- orthonormal polyanalytic polynomials
- orthonormal Laurent polynomials
- orthonormal rational functions
  [VB, Fasino, Gemignani, Mastronardi]

One-variable orthogonal polynomials

Basis functions: $p_j(z) = z^j$, $j = 0, 1, \ldots$.
Recurrence relation: $z[a_0(z), a_1(z), \ldots] = [a_0(z), a_1(z), \ldots]H$ with H upper Hessenberg
Hence: Computing (the recurrence relation coefficients of) the OPs $a_j(z)$ can be done by solving the following IEP.

Definition (IEP – one-variable OP)

Given: $D_z = \mathrm{diag}(z_i)$ – points, $\mathbf{w} = (w_i)$ – weights
Find: Unitary Q and upper Hessenberg H such that

$$Q^H \mathbf{w} = \|\mathbf{w}\| \mathbf{e}_1, \quad Q^H D_z Q = H.$$

[Boley, Golub]

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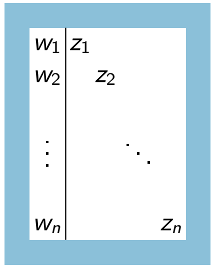
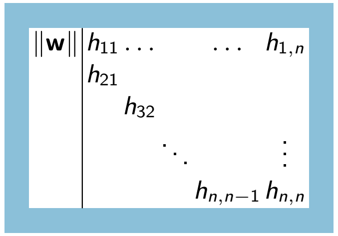
Algorithm for solving IEP – one-varaiable OP



→ sequence of unitary similarity transformations using Givens rotations →



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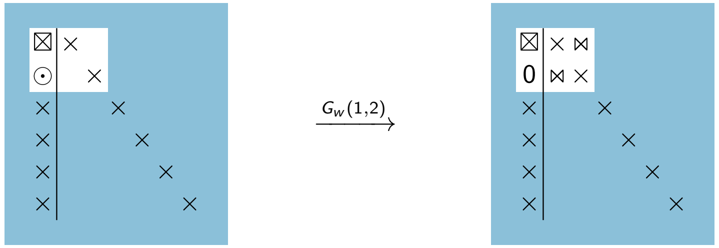
2 points



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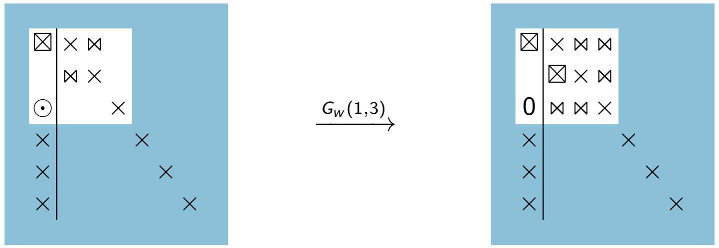
3 points (1)



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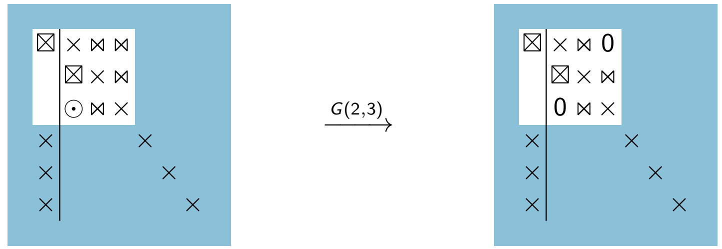

. . . skip some steps and jump to 6 points . . .

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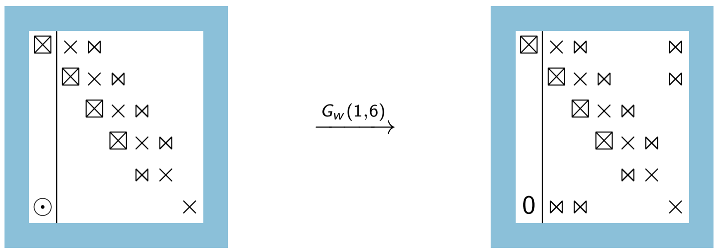
6 points (1)



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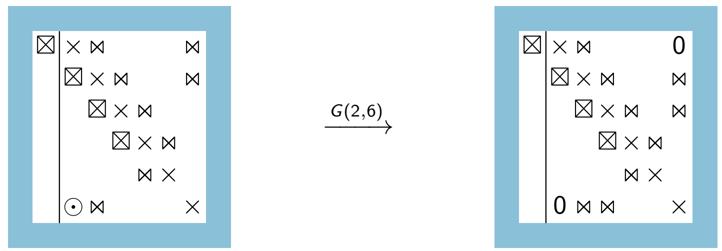
6 points (2)



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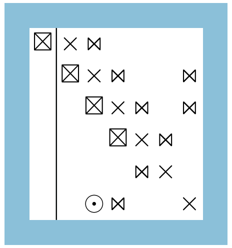
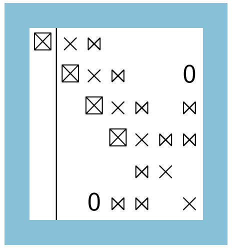
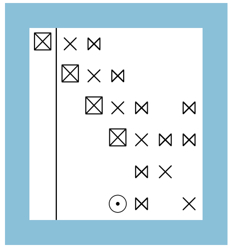
6 points (3)



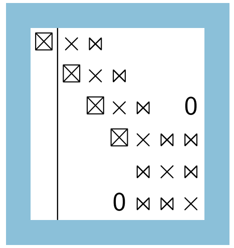
$\xrightarrow{G(3,6)}$



6 points (4)



$\xrightarrow{G(4,6)}$



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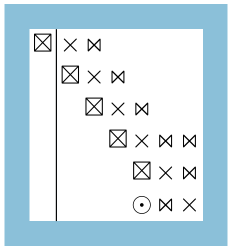
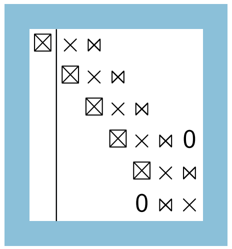
6 points (5)



$\xrightarrow{G(5,6)}$



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Computational complexity to solve the IEP

- in general: $\mathcal{O}(n^3)$ FLOPS
- w_i real, z_i real: $\mathcal{O}(n^2)$ FLOPS
- z_i on the complex unit circle: $\mathcal{O}(n^2)$ FLOPS using Schur parametrization, H is a unitary Hessenberg matrix

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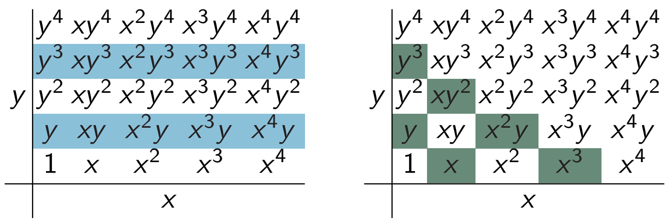
Two-variable orthogonal polynomials

Consider the monomials in two variables as basis functions $p_k(x,y) = x^i y^j$.

Choose an ordering of these basis functions such that:

- $xp_k(x,y) = p_m(x,y)$ with $m > k$
- $yp_k(x,y) = p_{m'}(x,y)$ with $m' > k$.

Two examples:



Define the inner product:

$$\langle p, q \rangle = \sum_{i=1}^{n} w_i^2 \overline{p(\xi_i, \eta_i)} q(\xi_i, \eta_i), \quad \xi_i, \eta_i \in \mathbb{R} \text{ or } \mathbb{C}.$$

Recurrence relation

Goal: Construct such a basis, generalizing one-var. algorithm

Idea: one-var. case: recurrence relation from multiplication by x:

$$x[a_0, a_1, \ldots, a_{n-1}] = [a_0, a_1, \ldots, a_{n-1}]H.$$

two-var. case: multiplications by x and y, separately:

$$x[a_1, a_2, \ldots, a_k, \ldots] = [a_1, a_2, \ldots, a_k, \ldots]H_x,$$
$$y[a_1, a_2, \ldots, a_k, \ldots] = [a_1, a_2, \ldots, a_k, \ldots]H_y.$$

H_x and H_y – generalized Hessenberg.

Some choice is left: i.e. $xy^2 = x \cdot y^2$ or $xy^2 = y \cdot xy$.

Recurrence coefficients: can be taken from the H_x or the H_y matrix.

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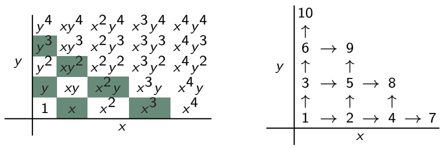
Example

We choose the following ordering:



leading to the following "recurrence relations" for the OP $a_i(z)$:

$$x[a_1(x,y), a_2(x,y), \ldots] = [a_1(x,y), a_2(x,y), \ldots]H_x$$
$$y[a_1(x,y), a_2(x,y), \ldots] = [a_1(x,y), a_2(x,y), \ldots]H_y$$

with the following "pivot" structure for H_x and H_y:

$$H_x = \begin{bmatrix} \times & \times & \times & \times & \cdots \\ \boxtimes & \times & \times & \times & \cdots \\ & \times & \times & \times & \cdots \\ & \boxtimes & \times & \times & \cdots \\ & & \boxtimes & \times & \cdots \\ & & & \times & \cdots \\ & & & \boxtimes & \cdots \\ & & & & \end{bmatrix} \qquad H_y = \begin{bmatrix} \times & \times & \times & \times & \cdots \\ \times & \times & \times & \times & \cdots \\ \boxtimes & \times & \times & \times & \cdots \\ & \times & \times & \times & \cdots \\ & \boxtimes & \times & \times & \cdots \\ & & \boxtimes & \times & \cdots \\ & & & \times & \cdots \\ & & & \boxtimes & \cdots \end{bmatrix}.$$

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Inverse eigenvalue problem

Computing (the recurrence relation coefficients of) the OPs $a_j(x,y)$ can be done by solving the following IEP.

Definition (IEP – two-variable OP)

Given: $D_x = \mathrm{diag}(x_i)$, $D_y = \mathrm{diag}(y_i)$ – points, $\mathbf{w} = (w_i)$ – weights

Find: Unitary Q and "generalized" upper Hessenberg matrices H_x and H_y such that

$$Q^H \mathbf{w} = \|\mathbf{w}\| \mathbf{e}_1, \quad Q^H D_x Q = H_x, \quad Q^H D_y Q = H_y$$

where the pivot structure of H_x and H_y determines the degree structure of the sequence of orthonormal polynomials.

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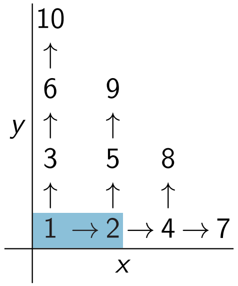
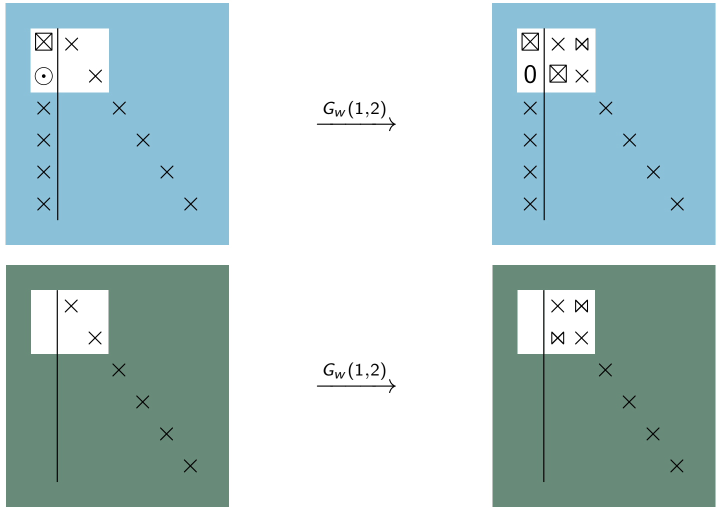
Order (2 points, 2 polynomials)



2 points



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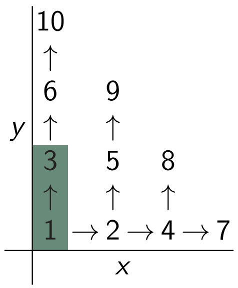
Order (3 points, 3 polynomials)



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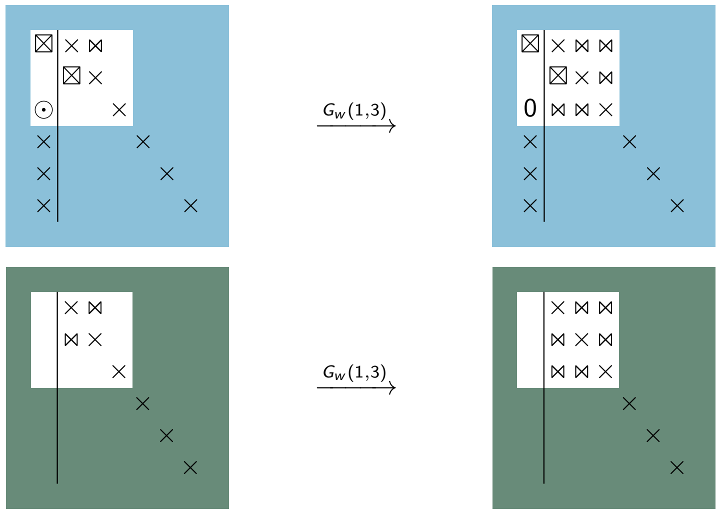
3 points (1)



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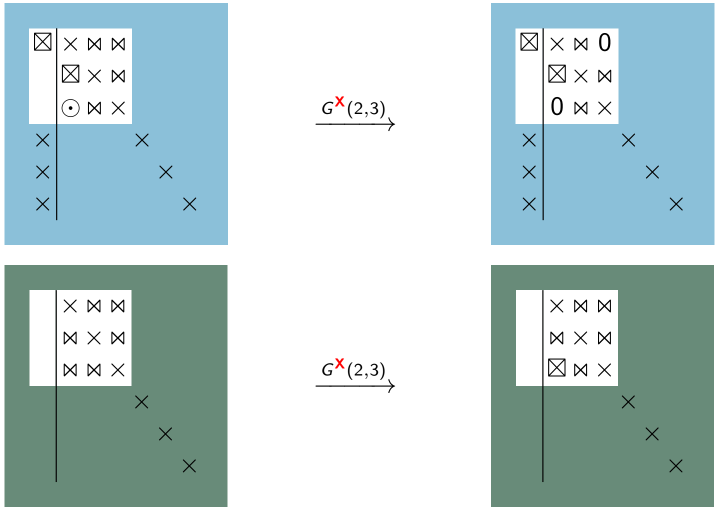
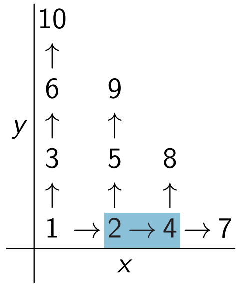
3 points (2)



Order (4 points, 4 polynomials)



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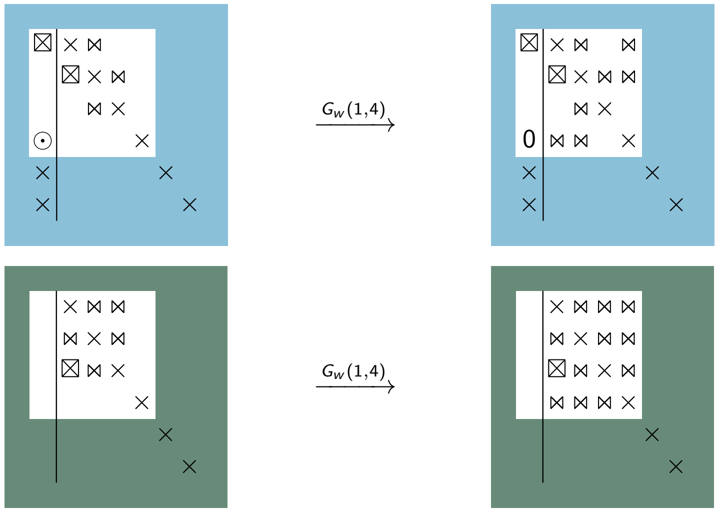
4 points (1)



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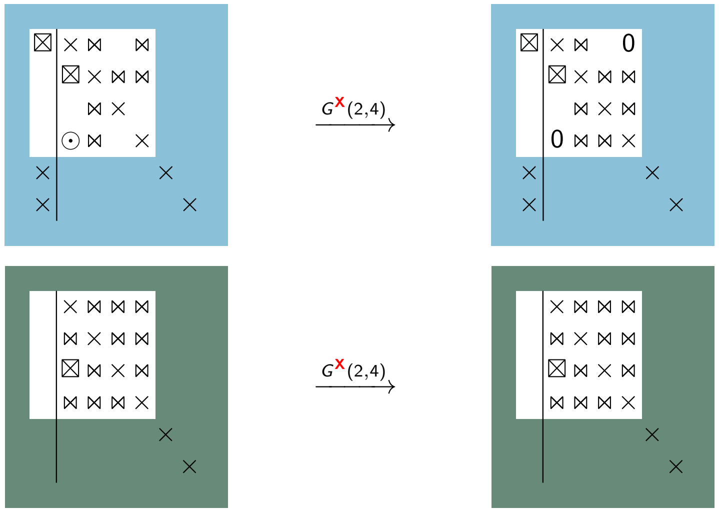
4 points (2)



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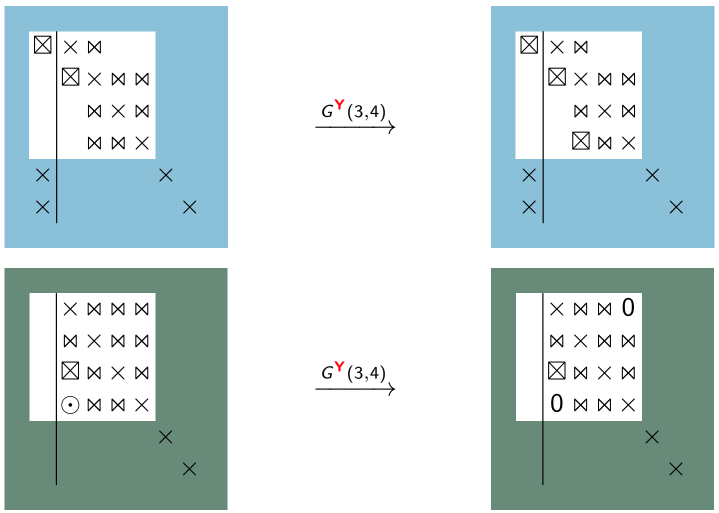
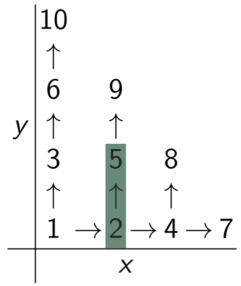
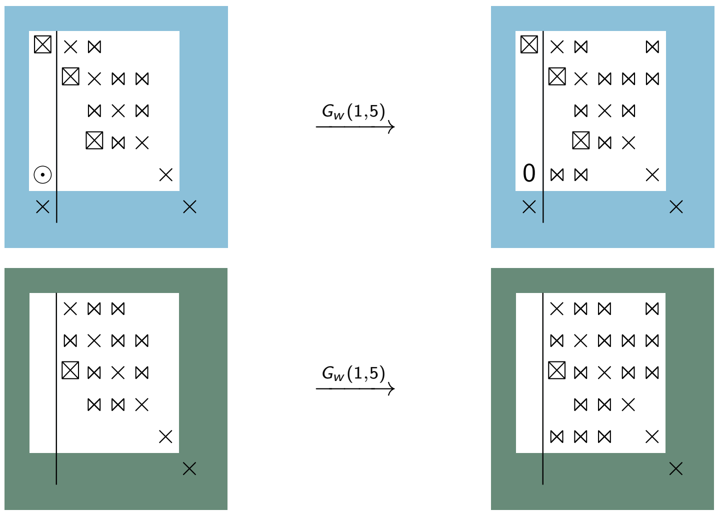
4 points (3)



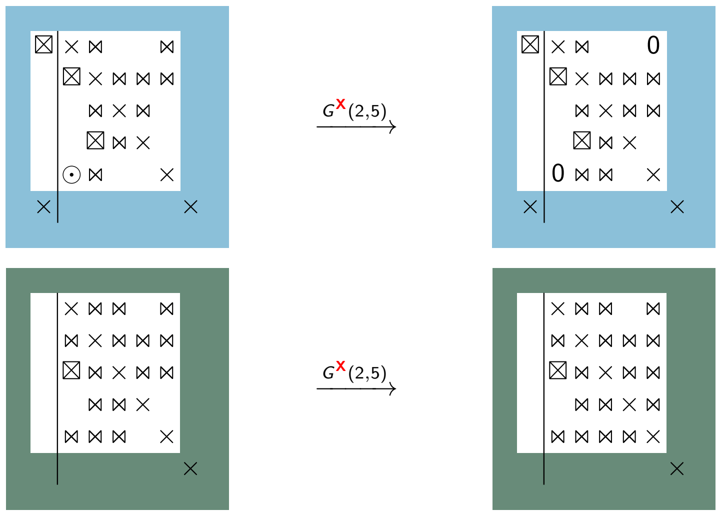
Order (5 points, 5 polynomials)



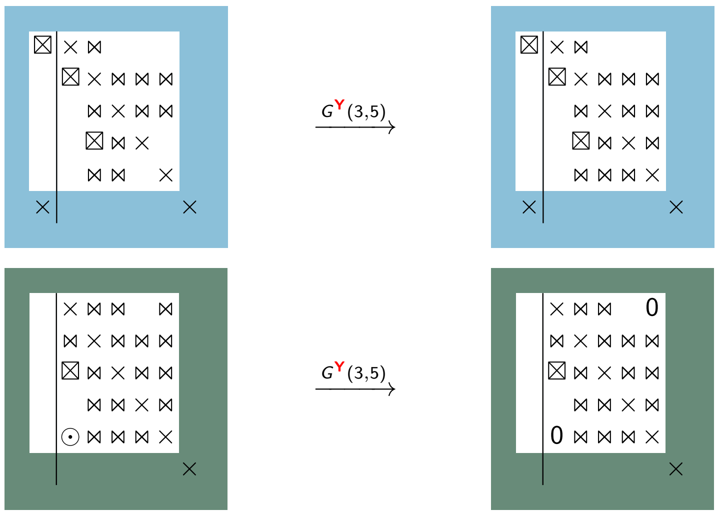
5 points (1)



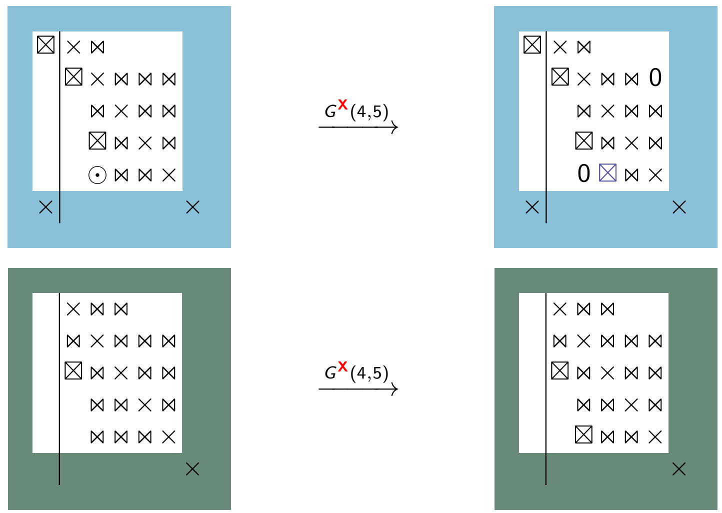
5 points (2)



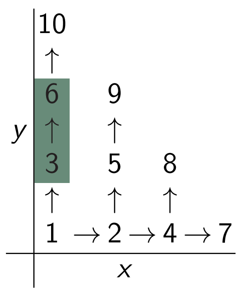
5 points (3)



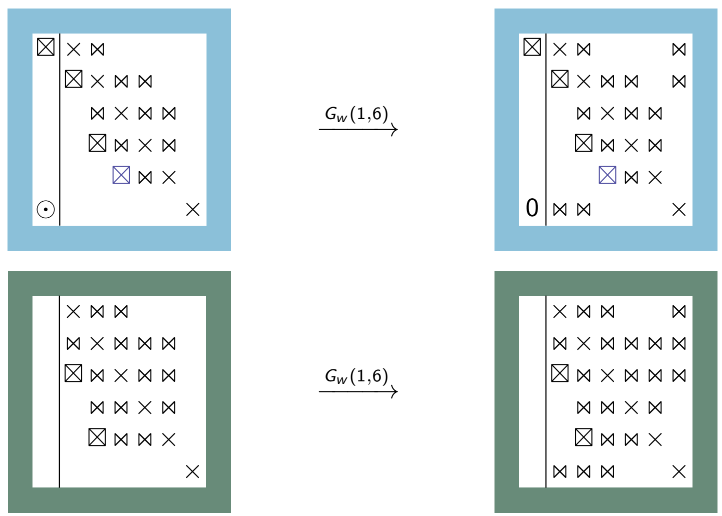
5 points (4)



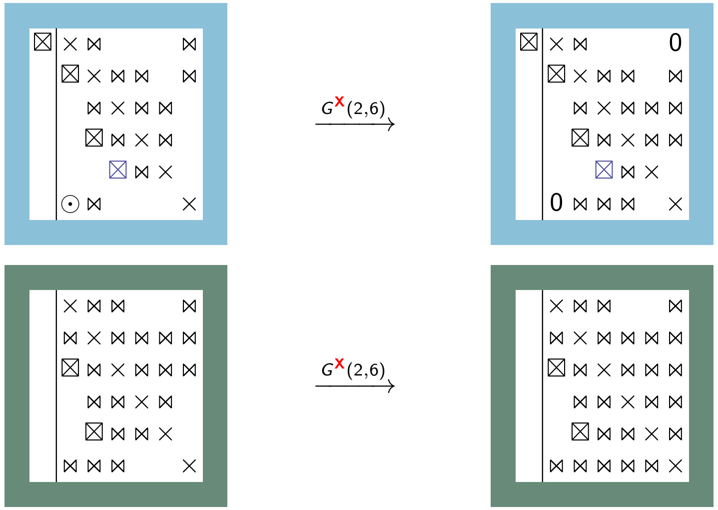
Order (6 points, 6 polynomials)



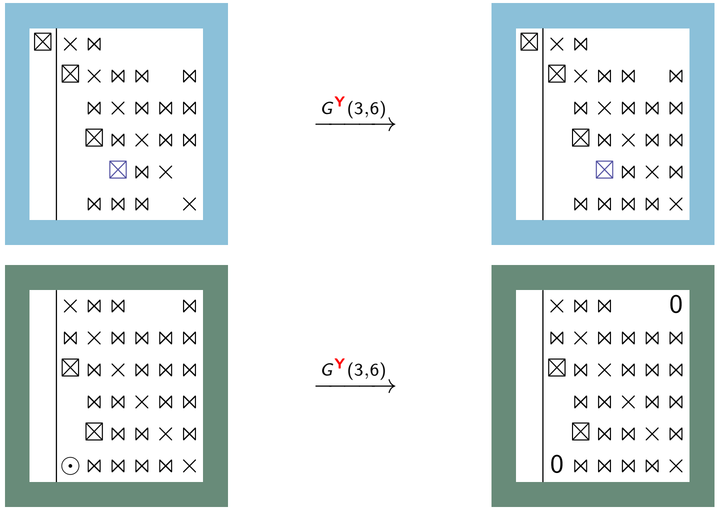
6 points (1)



6 points (2)



6 points (3)



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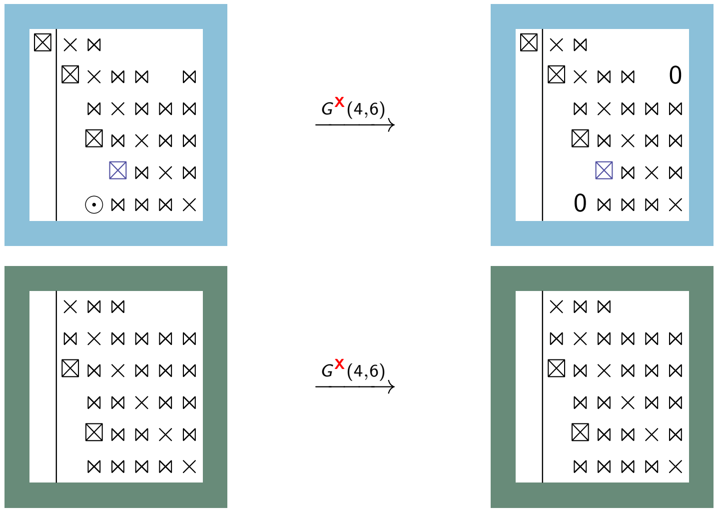
6 points (4)



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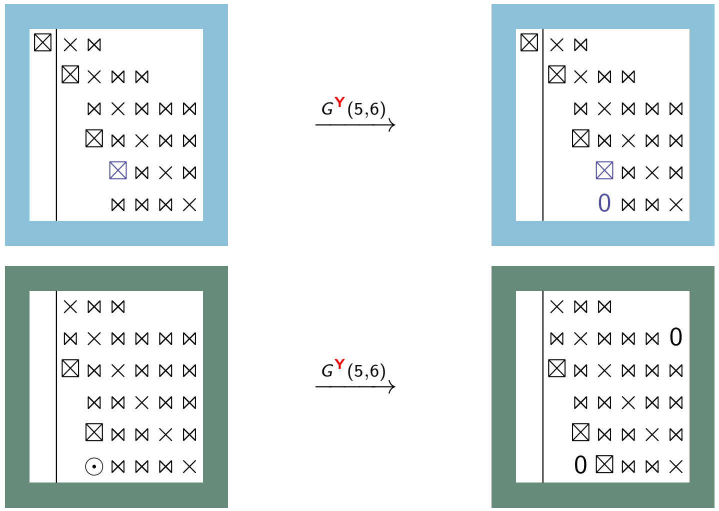
6 points (5)



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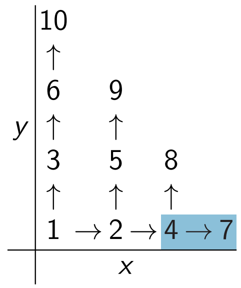
Recurrence relation

We can now recover the polynomials:

$$b_1 = const$$
$$xb_1 = [b_1, b_2] \cdot H_x(1:2,1)$$
$$yb_1 = [b_1, b_2, b_3] \cdot H_y(1:3,1)$$
$$xb_2 = [b_1, b_2, b_3, b_4] \cdot H_x(1:4,2)$$
$$yb_2 = [b_1, b_2, b_3, b_4, b_5] \cdot H_y(1:5,2)$$
$$xb_3 = [b_1, b_2, b_3, b_4, b_5] \cdot H_x(1:5,3)$$
$$yb_3 = [b_1, b_2, b_3, b_4, b_5, b_6] \cdot H_y(1:6,3)$$

More points, more polynomials...



and so on

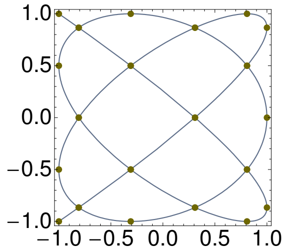
The Padua points as the inner product points

The $n = (\delta+1)(\delta+2)/2$ Padua points of degree δ are

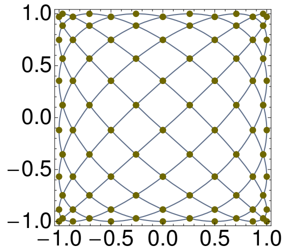
$$\mathrm{Pad}_\delta = \{\boldsymbol{\zeta} = (\zeta_1, \zeta_2)\} = \left\{ \gamma\left(\frac{k\pi}{\delta(\delta+1)}\right), \quad k = 0, \ldots, \delta(\delta+1) \right\}$$

where $\gamma(t)$ is their "generating curve"

$$\gamma(t) = (-\cos((\delta+1)t), -\cos(\delta t)) \quad t \in [0, \pi].$$



$\delta = 5$



$\delta = 13$

Example 1: Orthogonality test

Recall the IEP: Find unitary Q (transformation matrix) and generalized upper Hessenberg H_x and H_y such that $Q^H D_x Q = H_x$ and $Q^H D_y Q = H_y$.
Let $A = [a_1(\zeta_i)\, a_2(\zeta_i)\, \ldots\, a_n(\zeta_i)]_{i=1}^n$ and $W = \mathrm{diag}(w_i)$. Then $WA = Q$.

Test whether WA is orthogonal

- Take $n = 5151$ Padua points ζ_i of degree $\delta = 100$, $W = I$.
- Compute H_x, H_y.
- Compute values of OP's at all ζ_i's by recurrence relations stored in H_x, H_y. Multiply them with the corresponding weight w_i and store the results (columnwise) in $V = WA$. Let $R = |V^H V - I|$.
- For $k = 10:100:n$ compute $\max R(1:k, 1:k)$.

Example 1: Orthogonality test

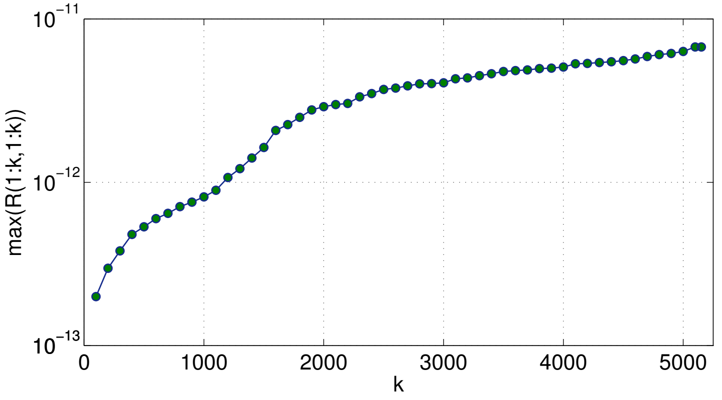


Figure: Max orthogonality error for the first k OPs, $n = 5151$ points

Example 2: Least squares test

Recall that the solution $p(z)$ to the discrete LS problem is

$$p(z) = \sum_{j=1}^{\alpha} c_j a_j(z).$$

Then $\mathbf{c} = (c_j)$ is given by $\mathbf{c} = A^H W^H W\mathbf{f} = [\langle a_i, \mathbf{f} \rangle]$, so we perform the same row operations on $W\mathbf{f}$ as on $\mathbf{w}$.

The LS solution

- Consider the Franke test function $F(\zeta)$ on $[0,1] \times [0,1]$ and transform the $n = 5151$ Padua points to fit $[0,1]^2$.
- Compute $\mathbf{f} = F(\zeta_i)$.
- Compute $A^H W^H W\mathbf{f} = \mathbf{c}$.
- Plot $|\mathbf{c}_k|$ for all k.

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Example 2: Least squares test

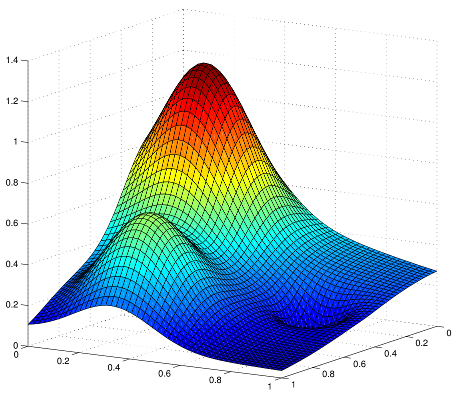

Figure: Franke function

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Example 2: Least squares test

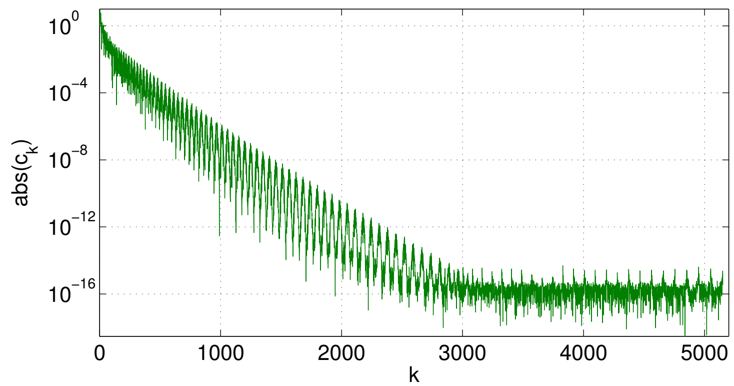

Figure: LS solution coefficients for Franke function, $n = 5151$ points

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Example 2: Least squares test, relative error

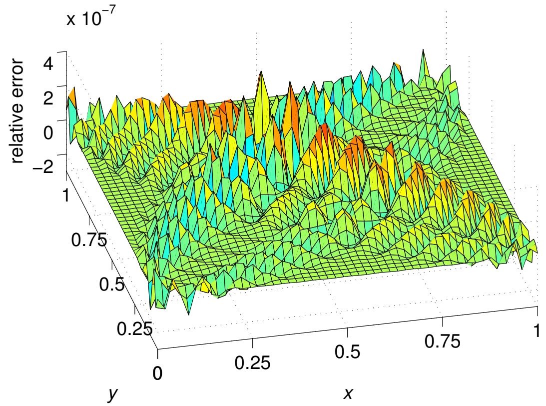

Figure: Relative error, appr poly of length 1000, $n = 5151$ points

Example 2: Least squares test, relative error

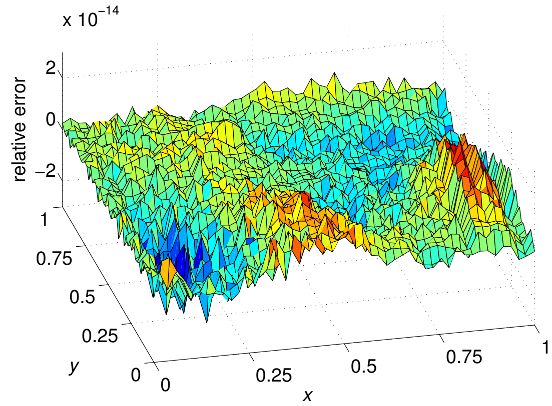

Figure: Relative error, appr poly of length 3000, $n = 5151$ points

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Example 3: Polynomial that goes through the points

Choice of the points

- Consider the square $[0, 1] \times [0, 1]$.
- 20 equidistant points on the circle with center $(0.25\ ;\ 0.25)$ and radius 0.15.
- The next 20 points similarly on a circle with center $(0.75\ ;\ 0.75)$.
- The last 4 points are the 4 corners of the square.

Find: the polynomial having “least degree” that has zero value in the given points.
Solution: look for the first zero pivot appearing in the recurrence relation.
This happens for the 28th orthogonal polynomial (of degree 6)

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Example 3: Polynomial that goes through the points

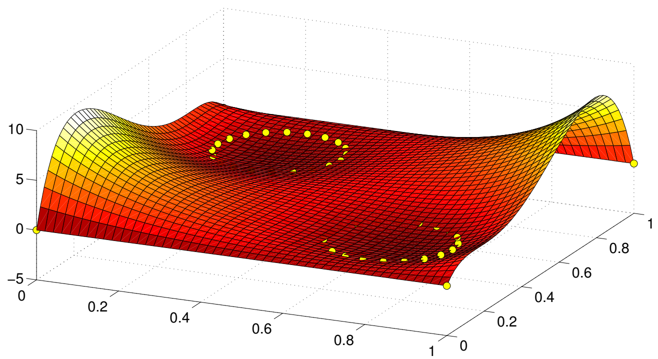

Figure: Surface plot of an interpolating polynomial

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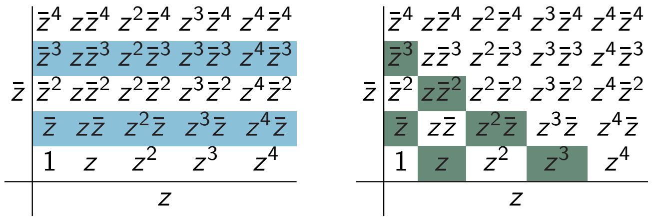
Orthogonal polyanalytic polynomials

Consider the monomials in the two variables z and $\bar{z}$ as basis functions $p_k(z,\bar{z}) = z^i \bar{z}^j$.

Choose an ordering of these basis functions such that:

- $zp_k(z,\bar{z}) = p_m(z,\bar{z})$ with $m > k$
- $\bar{z}p_k(z,\bar{z}) = p_{m'}(z,\bar{z})$ with $m' > k$.

Two examples:



Define the inner product:

$$\langle p, q \rangle = \sum_{i=1}^{n} w_i^2 \overline{p(z_i,\bar{z}_i)} q(z_i,\bar{z}_i), \quad z_i \in \mathbb{C}.$$

Recurrence relation

Goal: Construct such a basis, generalizing one-var. algorithm

Idea: one-var. case: recurrence relation from multiplication by z:

$$z[a_0, a_1, \ldots, a_{n-1}] = [a_0, a_1, \ldots, a_{n-1}]H.$$

two-var. case: multiplications by z and $\bar{z}$, separately:

$$z[a_1, a_2, \ldots, a_k, \ldots] = [a_1, a_2, \ldots, a_k, \ldots]H_z,$$
$$\bar{z}[a_1, a_2, \ldots, a_k, \ldots] = [a_1, a_2, \ldots, a_k, \ldots]H_{\bar{z}}.$$

H_z and $H_{\bar{z}}$ – generalized Hessenberg.

Some choice is left: i.e. $z\bar{z}^2 = z \cdot \bar{z}^2$ or $z\bar{z}^2 = \bar{z} \cdot z\bar{z}$.

Recurrence coefficients: can be taken from the H_z or the $H_{\bar{z}}$ matrix.

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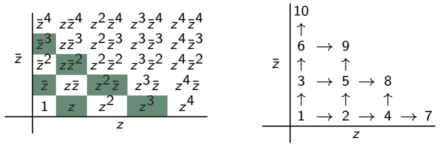
Example

We choose the following ordering:



leading to the following "recurrence relations" for the OP $a_i(z)$:

$$z[a_1(z,\bar{z}), a_2(z,\bar{z}), \ldots] = [a_1(z,\bar{z}), a_2(z,\bar{z}), \ldots]H_z$$
$$\bar{z}[a_1(z,\bar{z}), a_2(z,\bar{z}), \ldots] = [a_1(z,\bar{z}), a_2(z,\bar{z}), \ldots]H_{\bar{z}}$$

with the following "pivot" structure for H_z and $H_{\bar{z}}$:

$$H_z = \begin{bmatrix} \times & \times & \times & \times & \cdots \\ \boxtimes & \times & \times & \times & \cdots \\ & \times & \times & \times & \cdots \\ & \boxtimes & \times & \times & \cdots \\ & & \boxtimes & \times & \cdots \\ & & & \times & \cdots \\ & & & \boxtimes & \cdots \\ & & & & \end{bmatrix} \qquad H_{\bar{z}} = \begin{bmatrix} \times & \times & \times & \times & \cdots \\ \times & \times & \times & \times & \cdots \\ \boxtimes & \times & \times & \times & \cdots \\ & \times & \times & \times & \cdots \\ & \boxtimes & \times & \times & \cdots \\ & & \boxtimes & \times & \cdots \\ & & & \times & \cdots \\ & & & \boxtimes & \cdots \end{bmatrix}.$$

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Inverse eigenvalue problem

Computing (the recurrence relation coefficients of) the OPs $a_j(z,\bar{z})$ can be done by solving the following IEP.

Definition (IEP – two-variable OP)

Given: $D_z = \mathrm{diag}(z_i)$ – points, $\mathbf{w} = (w_i)$ – weights

Find: Unitary Q and "generalized" upper Hessenberg matrices H_z and $H_{\bar{z}}$ such that

$$Q^H\mathbf{w} = \|\mathbf{w}\|\mathbf{e}_1, \quad Q^H D_z Q = H_z, \quad Q^H D_{\bar{z}} Q = H_{\bar{z}}$$

where the pivot structure of H_z and $H_{\bar{z}}$ determines the degree structure of the sequence of orthonormal polynomials.

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Vector space of Laurent polynomials

Consider the vector space of Laurent polynomials $\mathcal{P}^\alpha = \{\sum_{i=1}^{\alpha} c_i p_i(z)\}$, with the sequence of basis functions $p_i(z)$:

$$1, z, z^{-1}, z^2, z^{-2}, z^3, z^{-3}, \ldots.$$

The leading index of a nonzero Laurent polynomial $p(z) = \sum_{i=1}^{\alpha} c_i p_i(z)$ is defined as

$$\text{l-index}(p) = \max\{i | c_i \neq 0\}.$$

Recurrence relation

Let us consider the leading indices of $za_i(z)$ and $z^{-1}a_i(z)$:

$$\text{l-index}(z[a_1(z), a_2(z), a_3(z), \ldots]) = [2, 4, \leq 4, 6, \leq 6, \ldots]$$
$$\text{l-index}(z^{-1}[a_1(z), a_2(z), a_3(z), \ldots]) = [3, \leq 3, 5, \leq 5, 7, \ldots].$$

This leads to the following "recurrence relations" for the OLP $a_i(z)$:

$$z[a_1(z), a_2(z), \ldots] = [a_1(z), a_2(z), \ldots]H_z$$
$$z^{-1}[a_1(z), a_2(z), \ldots] = [a_1(z), a_2(z), \ldots]H_{z^{-1}}$$

with the following "pivot" structure for H_z and $H_{z^{-1}}$:

$$H_z = \begin{bmatrix} \times & \times & \times & \times & \cdots \\ \boxtimes & \times & \times & \times & \cdots \\ & \times & \times & \times & \cdots \\ & \boxtimes & \times & \times & \cdots \\ & & & \times & \cdots \\ & & & \boxtimes & \cdots \\ & & & & \vdots \end{bmatrix} \qquad H_{z^{-1}} = \begin{bmatrix} \times & \times & \times & \times & \cdots \\ \times & \times & \times & \times & \cdots \\ \boxtimes & \times & \times & \times & \cdots \\ & & \times & \times & \cdots \\ & & \boxtimes & \times & \cdots \\ & & & & \vdots \end{bmatrix}.$$

Inverse eigenvalue problem

Computing (the recurrence relation coefficients of) the OLPs $a_j(z)$ can be done by solving the following IEP.

Definition (IEP – orthogonal Laurent polynomials)

Given: $Z = \text{diag}(z_i)$ – points, $\mathbf{w} = (w_i)$ – weights
Find: Unitary Q and "generalized" upper Hessenberg matrices H_z and $H_{z^{-1}}$ such that

$$Q^H\mathbf{w} = \|\mathbf{w}\|\mathbf{e}_1, \quad Q^H Z Q = H_z, \quad Q^H Z^{-1} Q = H_{z^{-1}}$$

where the pivot structure of H_z and $H_{z^{-1}}$ determines the degree structure of the sequence of orthonormal Laurent polynomials.

Vector space

Given the complex numbers $y_1, y_2, \ldots, y_n$ all different from each other. Let us consider the vector space $\mathcal{P}^n$ of all proper rational functions having possible poles in $y_1, y_2, \ldots, y_n$:

$$\mathcal{P}^n = \text{span}\{1, \frac{1}{z - y_1}, \frac{1}{z - y_2}, \ldots, \frac{1}{z - y_n}\}.$$

Bilinear form

Given the complex numbers $z_0, z_1, \ldots, z_n$ which together with the numbers y_i are all different from each other, and the "weights" $0 \leq w_i$, $i = 0, 1, \ldots, n$, we define the following bilinear form

$$\langle p, q \rangle = \sum_{i=0}^{n} w_i^2 \overline{p(z_i)} q(z_i).$$

This bilinear form defines an inner product in the space $\mathcal{P}^n$.

Orthonormal basis

Let us consider an orthonormal basis

$$\mathbf{a}_n = [a_0, a_1, \ldots, a_n]$$

for $\mathcal{P}^n$ satisfying the following properties

$$a_j \in \mathcal{P}^j \setminus \mathcal{P}^{j-1} \qquad (\mathcal{P}^{-1} = \emptyset)$$
$$\langle a_i, a_j \rangle = \delta_{i,j} \qquad \text{(Kronecker delta)}$$

for $i, j = 0, 1, 2, \ldots, n$.

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Recurrence relation

The recurrence relation for the orthonormal rational functions $a_j(z)$ for $j = 0, 1, \ldots, n$ can be written as:

$$\mathbf{a}(z)(zI - D_y)H = \mathbf{a}(z) + c a_{n+1}(z)\mathbf{e}_n$$

with $a_{n+1}(z) = \frac{\prod_{j=0}^{n}(z - z_j)}{\prod_{j=1}^{n}(z - y_j)}$ and $D_y = \mathrm{diag}(y_0, y_1, \ldots, y_n)$ with y_0 chosen arbitrarily.
Multiply to the right by the inverse of the upper Hessenberg matrix H: $S = H^{-1}$:

$$z\mathbf{a}(z) = \mathbf{a}(z)(S + D_y) + c a_{n+1}(z)\mathbf{s}_n$$

with $\mathbf{s}_n$ the last row of the matrix S.
Note that the matrix S is lower semiseparable, i.e., has rank 1 structure in the lower triangular part: $tril(S) = tril(\text{rank 1 matrix})$.

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Connecting the ORF $a_j(z)$ to the columns of Q

Recurrence relation for $a_j(z)$:

$$z\mathbf{a}(z) = \mathbf{a}(z)(S + D_y) + c a_{n+1}(z)\mathbf{s}_n$$

with $a_{n+1}(z) = \frac{\prod_{j=0}^{n}(z - z_j)}{\prod_{j=1}^{n}(z - y_j)}$.
Because

$$Q_j = [w_i a_j(z_i)]_{i=0,1,\ldots,n}$$

we derive the following relation for the unitary matrix Q:

$$D_z Q = Q(S + D_y), \qquad \text{or} \qquad Q^H D_z Q = S + D_y.$$

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Construction of the basis

Solve the following inverse eigenvalue problem:

Definition (IEP – orthogonal rational functions)

Given: $D_z = \mathrm{diag}(z_i)$, $D_y = \mathrm{diag}(y_i)$ – points, poles, $\mathbf{w} = (w_i)$ – weights

Find: Unitary Q and lower-semiseparable matrix S such that

- $Q^H D_z Q = S + D_y$ with Q unitary
- the first component of the normalised eigenvector corresponding to z_i equals $w_i/\|\mathbf{w}\|$, i.e., $Q^H\mathbf{w} = \mathbf{e}_1\|\mathbf{w}\|$
- $\mathrm{tril}(S) = \mathrm{tril}(\text{rank 1 matrix})$

Recurrence relation

Later on we will design an algorithm to compute Q and S. Now we will look at a recurrence relation between the columns Q_j of Q. Then we will give the connection between the columns Q_j and the values of rational functions satisfying a similar recurrence relation. Finally, we will show that these rational functions form a basis we are looking for.
notation: $H = S^{-1}$ is upper Hessenberg with subdiagonal elements $b_0, b_1, \ldots, b_{n-1}$. The jth column H_j of H has the form

$$H_j^T =: [\vec{h}_j^T, b_j, \vec{0}^T].$$

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Recurrence relation for Q_j

Let $Q =: [Q_0, Q_1, \ldots, Q_n]$.
The columns Q_j satisfy the following recurrence relation

$$\begin{aligned} (D_z - y_{j+1}I)b_j Q_{j+1} &= Q_j \\ &+ ([Q_0, Q_1, \ldots, Q_j]\, D_{y,j} - D_z\, [Q_0, Q_1, \ldots, Q_j])\, \vec{h}_j \\ j &= 0, 1, \ldots, n-1 \end{aligned}$$

with

$$Q_0 = \frac{\mathbf{w}}{\|\mathbf{w}\|}$$

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Proof

Because $Q^H\mathbf{w} = \mathbf{e}_1\|\mathbf{w}\|$, it follows that $Q_0 = \frac{\mathbf{w}}{\|\mathbf{w}\|}$.
Multiplying $Q^H D_z Q = S + D_y$ to the left by Q, leads to

$$D_z Q = Q(S + D_y).$$

Multiplying this to the right by $H = S^{-1}$, gives us

$$D_z Q H = Q(I + D_y H).$$

Considering the jth column from the left and right-hand side gives us the recurrence relation:

$$\begin{aligned} (D_z - y_{j+1}I)b_j Q_{j+1} &= Q_j \\ &+ ([Q_0, Q_1, \ldots, Q_j]\, D_{y,j} - D_z\, [Q_0, Q_1, \ldots, Q_j])\, \vec{h}_j \\ j &= 0, 1, \ldots, n-1. \end{aligned}$$

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Recurrence relation

Looking at the recurrence relation for Q_j

$$(D_z - y_{j+1} I) b_j Q_{j+1} = Q_j + \left([Q_0, Q_1, \ldots, Q_j]\, D_{y,j} - D_z \,[Q_0, Q_1, \ldots, Q_j] \right) \vec{h}_j$$
$$j = 0, 1, \ldots, n-1$$

we can compute an orthonormal basis $[a_0, a_1, \ldots, a_n]$ for $\mathcal{P}^n$ using a similar recurrence relation

$$a_{j+1}(z) = \frac{a_j(z) + \left([a_0, a_1, \ldots, a_j]\, D_{y,j} - z\,[a_0, a_1, \ldots, a_j] \right) \vec{h}_j}{(z - y_{j+1}) b_j},$$

for $j = 0, 1, \ldots, n-1$ and
with $a_0(x) = 1/\sqrt{\sum |w_i|^2}$.

Theorem

For $j = 0, 1, \ldots, n$ we have that

$$Q_j = \operatorname{diag}(\mathbf{w})\,[a_j(z_i)]$$
$$a_j \in \mathcal{P}^j \setminus \mathcal{P}^{j-1}$$

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Proof

Filling in z_i for z in the recurrence relation for $a_{j+1}(z)$, we get

$$(D_z - y_{j+1} I) b_j \,[a_{j+1}(z_i)] = a_j(z_i) + [a_0(z_i), a_1(z_i), \ldots, a_j(z_i)]\, D_{y,j} \vec{h}_j - D_z\,[a_0(z_i), a_1(z_i), \ldots, a_j(z_i)]\, \vec{h}_j.$$

Because $Q_0 = \operatorname{diag}(\mathbf{w})\,[a_0(z_i)]$ and because $\operatorname{diag}(\mathbf{w})$ is diagonal as well as all the other square matrices involved, first part of the theorem is proved.

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Proof (continued)

We have to prove that $a_j \in \mathcal{P}^j \setminus \mathcal{P}^{j-1}$.
This is clearly true for $j = 0$.
Suppose it is true for $j = 0, 1, 2, \ldots, k < n$.
From the recurrence relation, we derive that $a_{k+1}(z)$ has the form

$$a_{k+1}(z) = \frac{\text{rat. function with possible poles in } y_0, y_1, \ldots, y_k}{(z - y_{j+1})}.$$

Also $\lim_{z \to \infty} a_{k+1}(z) \in \mathbb{C}$.
Hence, $a_j \in \mathcal{P}^j \setminus \mathcal{P}^{j-1}$.

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Orthonormality of $\vec{a}_n$

The functions $\vec{a}_n = [a_0, a_1, \ldots, a_n]$ form an orthonormal basis for $\mathcal{P}^n$ with respect to the inner product $\langle \cdot, \cdot \rangle$. Moreover, $\_i \in \mathcal{P}^i \setminus \mathcal{P}^{i-1}$.
Proof The only thing that remains to be proven is $\langle a_i, a_j \rangle = \delta_{i,j}$. This follows immediately from the fact that $Q = \mathrm{diag}(\mathbf{w}) \left[a_j(z_i)\right]$ and Q is unitary.

Recurrence relation

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$$z\mathbf{a}(z) = \mathbf{a}(z)(S + D_y) + c a_{n+1}(z)\mathbf{s}_n$$

with $\mathbf{s}_n$ the last row of the semiseparable matrix S and $a_{n+1}(z) = \frac{\prod_{j=0}^{n}(z-z_j)}{\prod_{j=1}^{n}(z-y_j)}$.

Proof

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The recurrence relation for the a_j, $j = 0, 1, \ldots, n$ can also be written as

$$\mathbf{a}(z)(zI - D_y)H = \mathbf{a}(z) + c a_{n+1}(z)\mathbf{e}_n.$$

Multiplying to the right by $S = H^{-1}$, we derive the recurrence formula.
To determine a_{n+1} we look at the last column of the previous relation. It follows that a_{n+1} is a rational function having degree of numerator at most one more than the degree of the denominator and having possible poles in $y_1, y_2, \ldots, y_n$.

Proof (continued)

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Let us evaluate the previous equation in the points z_i

$$D_z \left[a_j(z_i)\right] H - \left[a_j(z_i)\right] D_y H = \left[a_j(z_i)\right] + c \left[a_{n+1}(z_i)\right] \mathbf{e}_n.$$

Multiplying to the left by $\mathrm{diag}(\mathbf{w}) = D_w$ and because $D_w D_z = D_z D_w$, we obtain

$$D_z Q H - Q D_y H = Q + c D_w \left[a_{n+1}(z_i)\right] \mathbf{e}_n.$$

From

$$D_z Q H = Q(I + D_y H)$$

it follows that a_{n+1} has zeros in z_i, $i = 0, 1, \ldots, n$ and this proves the theorem.

Note

Note that a_{n+1} is orthogonal to all a_i, $i = 0, 1, 2, \ldots, n$.
The norm squared is

$$\|a_{n+1}\|^2 = \langle a_{n+1}, a_{n+1} \rangle = 0.$$

Special cases

- if all z_i and y_i are real: $Q^T D_z Q = S + D_y$
  Hence, S is symmetric.
- if all z_i are real but y_i can be complex then the strictly upper triangular part R is also of rank 1.
- if z_i are all on the unit circle, then the strictly upper triangular part R is also of rank 1.

In all these cases the computational complexity reduces to $\mathcal{O}(n^2)$.

Connection between Q, H and the OPs

Consider the following recurrence relation for b_i:

$$b_0 = \frac{1}{\|\mathbf{w}\|}, \quad z[b_0, b_1, \ldots, b_{n-1}] = [b_0, b_1, \ldots, b_{n-1}]H. \qquad (2)$$

H Hessenberg $\Rightarrow$ derive b_1 from 1st col, b_2 from 2nd, ...

$$Q^H \mathbf{w} = \|\mathbf{w}\| \mathbf{e}_1 \quad \Rightarrow \quad Q\mathbf{e}_1 = \frac{\mathbf{w}}{\|\mathbf{w}\|} = \mathrm{diag}(\mathbf{w})[b_0(z_i)]$$

$$D_z Q = QH \quad \Rightarrow \quad Q\mathbf{e}_k = \mathrm{diag}(\mathbf{w})[b_{k-1}(z_i)],\ k = 1, 2, \ldots, n.$$

Since $Q^H Q = I$, we have that:
(1) b_i are OPs wrt (1), (2) $a_i = b_i$ and thus (3) $WA = Q$
with $W = \mathrm{diag}(w_i)$ and $A_{i,j} = [a_j(z_i)]$.

Vector case of discrete LS approximation

Discrete vector LS approximation

Given: L functions $f_j(z)$, $z \in \mathcal{D} \subset \mathbb{C}$, N points $z_i \in \mathcal{D} \subset \mathbb{C}$ and corresponding weights w_i
Find: L polynomials $p_j(z)$: $\deg p_j \leqslant \alpha_j$ and a normalization s.t.

$$\sum_{i=1}^{N} w_i^2 \left| \begin{bmatrix} f_1 \ f_2 \cdots f_L \end{bmatrix} \begin{bmatrix} p_1 \\ \vdots \\ p_L \end{bmatrix} \right|_{z=z_i} \quad |^2 \quad \text{is minimal.}$$

Special case: discrete LS approximation

Find: the polynomial $p(z)$ of degree $\leqslant \alpha$ s.t.

$$\sum_{i=1}^{N} w_i^2 |f(x_i) - p(z_i)|^2 = \sum_{i=1}^{N} w_i^2 | \begin{bmatrix} f(z_i) & -1 \end{bmatrix} \begin{bmatrix} 1 \\ p(z_i) \end{bmatrix} |^2 \quad \text{is min.}$$

[VB, Bultheel]