Applications of Orthogonal rational functions

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Part I: Orthogonal rational functions (ORF)

1. Orthogonal polynomials vs rational functions
   - Orthogonal polynomials
   - Orthogonal rational functions
   - Least squares
   - Minimax

Outline of Part II: Applications

2 The linear prediction problem
3 System identification
4 Spectral methods for ODE/PDE
5 Fast algorithms for structured matrices
6 Krylov subspace iteration
7 Rational Szegő quadrature

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Part I

Orthogonal rational functions

Orthogonal polynomials (OP)

- Obtained by orthogonalization of $\{1, z, z^2, \ldots\}$
- On $\mathbb{R}$, $[0, \infty)$, $[a, b]$, $\mathbb{T}$
- With respect to some measure $\langle f, g \rangle = \int f(z)\overline{g(z)}d\mu(z)$
- $\operatorname{span}\{z^k\}_{k=0}^n = \mathcal{L}_n \subset L^2(\mu)$ is finite dimensional subspace
- Infinite dimensional problem in L^2 approximated in finite dimensional subspace $\mathcal{L}_n$

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Orthogonal rational functions (ORF)

- OP in z = ORF with all poles at infinity ...
  or OP in z^{-1} = ORF with all poles in the origin.
- Fix a sequence of poles: $\{\alpha_1, \alpha_2, \ldots\}$
  usually in some subset of $\mathbb{C} \cup \{\infty\}$
  possibly in $\mathbb{R}$ or outside $[a, b]$,
  inside or outside the support of μ,...
- Obtained by orthogonalization of $\{1, \frac{1}{z-\alpha_1}, \frac{1}{(z-\alpha_1)(z-\alpha_2)}, \ldots\}$
- $\operatorname{span}\{\frac{z^k}{(z-\alpha_1)\cdots(z-\alpha_n)}\}_{k=0}^{n} = \mathcal{L}_n \subset L^2(\mu)$ is finite dimensional subspace
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Orthogonal rational functions

Most of what holds for OP can be generalized to ORF.

$$\mathcal{L}_n = \operatorname{span}\{\phi_0, \phi_1, \ldots, \phi_n\}, \quad \langle \phi_k, \phi_l \rangle = \delta_{kl}$$

- Recurrence relations (3-term for part of real line, Szegő for $\mathbb{T}$)
- Reproducing kernels $k_n(z, w) = \sum_{k=0}^{n} \phi_k(z)\overline{\phi_k(w)}$

$$\langle f, k_n(\cdot, w) \rangle = f(w), \quad \forall f \in \mathcal{L}_n$$

- Christoffel-Darboux relations $k_n(z, w) = F(\phi_n) = \tilde{F}(\phi_{n+1})$
- Moment problems: given $M(\mu) = [\mu_{ij} = \langle b_i, b_j \rangle]$, find μ
- Quadrature formulas: $\forall f, g \in \mathcal{L}_n$

$$\langle f, g \rangle_{\mu_n} = \sum w_i f(z_i)\overline{g(z_i)} = \langle f, g \rangle_{\mu} = \int f(z)\overline{g(z)} d\mu(z).$$

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Least squares

For any subspace $\mathcal{L}_n = \operatorname{span}\{\phi_0, \ldots, \phi_n\} \subset L^2(\mu)$ with Orthogonal Basis ϕ_i holds:

- If $f = \sum_{k=0}^{\infty} c_k \phi_k \in L^2(\mu)$ then the best least squares approximant in $\mathcal{L}_n = \operatorname{span}\{\phi_0, \ldots, \phi_n\}$ is given by truncation: $f_n = \sum_{k=0}^{n} c_k \phi_k$ with $c_k = \langle f, \phi_k \rangle$ and $\|f - f_n\|$ is min.
- Among all $f \in \mathcal{L}_n$ the one with minimal $L^2(\mu)$ norm satisfying $f(w) = 1$ is $k_n(z, w)/k_n(w, w)$ and the min is $1/k_n(w, w)$.

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Minimax approximation

For any subspace $\mathcal{L}_n = \operatorname{span}\{\phi_0, \ldots, \phi_n\}$ of rational functions defined on $[-1, 1]$ with poles in $A = \{\alpha_1, \ldots, \alpha_n\}$

- Let $f_n \in \mathcal{L}_n$ be an interpolant to f in the points $X = \{x_0, \ldots, x_n\}$ with $A \cap X = \varnothing$.
- Then $\exists c \in [-1, 1]$ such that

$$|f - f_n| = \frac{|(f\pi)^{(n+1)}(c)|}{(n+1)!} \prod_{k=0}^{n} \frac{|x - x_k|}{|x - \alpha_k|}$$

- Thus it is important to minimize $\max \prod_k \frac{|x-x_k|}{|x-\alpha_k|}$.
- $\therefore$ choose x_i as the zeros of an equioscillating $\phi \in \mathcal{L}_n$.
  A *Chebyshev* ORF orthogonal with respect to $1/\sqrt{1-x^2}$.

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Part II

Applications

Stochastic process

- $\{y_n\}_{n\in\mathbb{Z}}$, sequence of stochastic variables
- $\mu_k = \mathrm{E}\{y_n \overline{y}_{n-k}\}$ stationary (time invariant)
- $\hat{y}_n = -\sum_{k=1}^{\infty} a_k y_{n-k}$ predict from past
- in $\mathrm{span}\{y_k\}$ is $\mathrm{E}\{x\overline{y}\}$ an inner product
- $\Leftrightarrow L_2(\mathbb{T},\mu)$ with $\langle f, g\rangle = \int f(t)\overline{g(t)}d\mu(t)$
- μ is spectral measure (μ_k are the trigonometric moments of μ)
- $y_k \leftrightarrow z^{-k}$, $H_2^+ = \mathrm{span}\{z^k : k \geq 1\}$ = past of y_0
- minimize energy $\|e_n\|^2$, $e_n = y_n - \hat{y}_n = \sum_{k=0}^{\infty} a_k y_{n-k}$, $a_0 = 1$
- $\Leftrightarrow$ project 1 onto H_2^+ in $L_2(\mathbb{T},\mu)$

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- $\hat{y}_n = -\sum_{k=1}^{\infty} a_k y_{n-k}$ predict from past
- in span$\{y_k\}$ is $\mathrm{E}\{x\overline{y}\}$ an inner product
- $\Leftrightarrow$ $L_2(\mathbb{T},\mu)$ with $\langle f, g\rangle = \int f(t)\overline{g(t)}d\mu(t)$
- μ is spectral measure (μ_k are the trigonometric moments of μ)
- $y_k \leftrightarrow z^{-k}$, $H_2^+ = \mathrm{span}\,\{z^k : k \geq 1\}$ = past of y_0
- minimize energy $\|e_n\|^2$, $e_n = y_n - \hat{y}_n = \sum_{k=0}^{\infty} a_k y_{n-k}$, $a_0 = 1$
- $\Leftrightarrow$ project 1 onto H_2^+ in $L_2(\mathbb{T},\mu)$

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Take n-dimensional subspaces of H_2^-

- project 1 onto $\text{span}\{z^k, k = 1, \ldots, n\} \Rightarrow \min_{p_n} \|p_n\|_\mu^2$, $p_n(z) = 1 + a_1 z + \ldots + a_n z^n$
- But if predictor is $1 + az + a^2 z^2 + \cdots + a^n z^n + \cdots = 1/(1 - az)$ and $|a|$ is close to 1, then coefficients will decay very slowly and need a predictor polynomial of a high degree.
- Better to look for $\min_{p_n} \|p_n\|_\mu^2$, $p_n(0) = 1$, $p_n \in \mathcal{L}_n$ with $\mathcal{L}_n = \text{span}\{1, 1/(1 - az), 1/(1 - az)^2, \ldots, 1/(1 - az)^n\}$ or more generally $\mathcal{L}_n = \text{span}\left\{1, \frac{1}{\pi_1}, \frac{1}{\pi_2}, \ldots, \frac{1}{\pi_n}\right\}$, $\pi_k(z) = \prod_{j=1}^k (1 - a_j z)$
- ORF on $\mathbb{T}$
- Solution is $p_n(z) = k_n(z, 0)/k_n(0, 0)$ and $\min = 1/k_n(0, 0)$.

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Linear system: input-output description

- Discrete time linear stationary system $y(t) = h(t) * u(t)$
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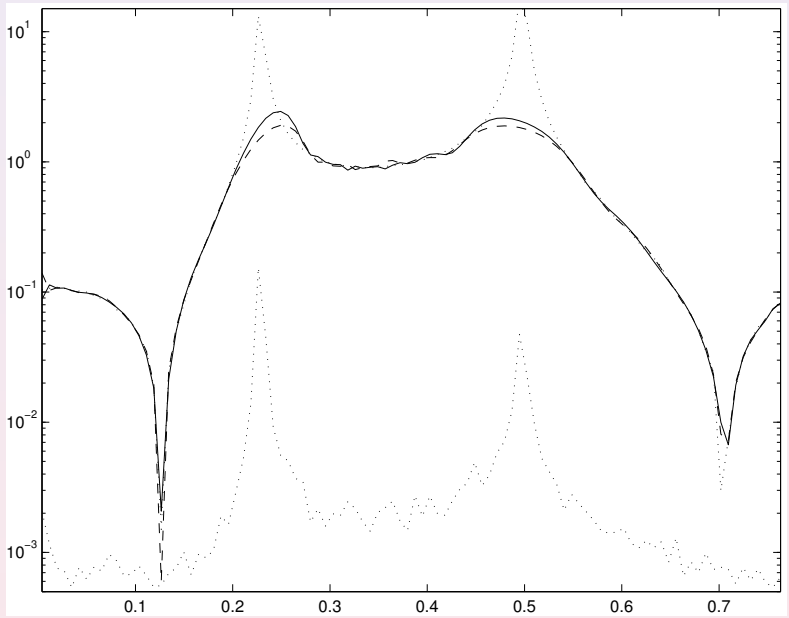
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Example: Robot arm



$N = 100$ measurements
Uncertainties = lower dotted line.
Measured system = upper dotted line.
Peaks in spectrum predict the location of the poles.
Approximation = full line with 2 pairs of complex conjugate poles repeated 7 times, hence a degree 28 approximation.

Numerical techniques for PDE/ODE

Consider a PDE

$$Lu(x) = s(x), \quad x \in U \subset \mathbb{R}^d \tag{1}$$
$$Bu(x) = 0, \quad x \in \partial U \tag{2}$$

L, B linear differential operators.
Solve approximately by satisfying (2) and minimizing $R = Lu - s$.

- finite differences: approximate L, B with local polynomials
- finite elements: approximate u with local supported elements
- spectral methods: via Fourier transform

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$$Lu(x) = s(x), \quad x \in U \quad \text{and} \quad Bu(x) = 0, \quad x \in \partial U.$$

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- $\langle \chi_k, R \rangle = 0$, $k = 0, \ldots, N$, $\{\chi_k\}$ test functions
  (make 'small' for space spanned by test fct.)

3 spectral methods

- Galerkin: $\chi_k = \phi_n$ and $B\phi_k = 0$
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Collocation = Pseudospectral method

$$R(x) = Lu(x) - s(x) = 0, \quad x \in U \quad \text{and} \quad Bu(x) = 0, \quad x \in \partial U.$$

$\langle \chi_k, R \rangle = 0$ means approximant (= projection onto $\operatorname{span}\{\phi_k\}$)

$$P_N(u) = \tilde{u}(x) = \sum_{k=0}^{N} \tilde{u}_k \phi_k(x), \quad \tilde{u}_k = \frac{\langle \phi_k, u \rangle}{\langle \phi_k, \phi_k \rangle},$$

$L\tilde{u}$ should interpolate s in the points x_k, $k = 0, \ldots, N$.
Minimize max interpolation error *independent of* f means minimizing $\prod |x - x_i|$ (polynomial) or $\prod \frac{|x-x_i|}{|x-\alpha_i|}$ (rational).
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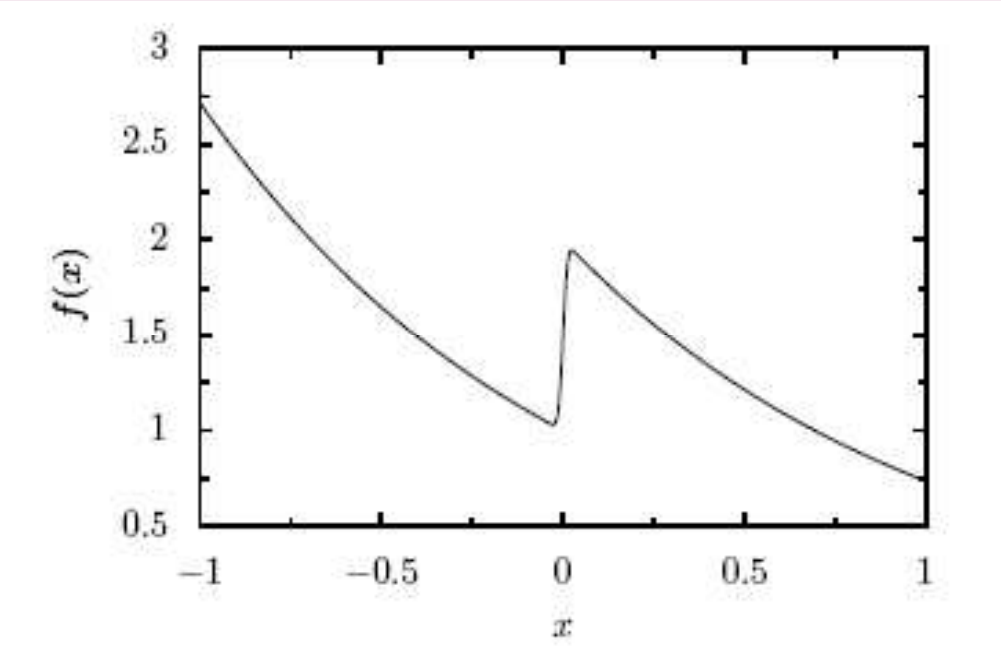
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Example of ODE

$$\varepsilon f''(x)+xf'(x)+xf(x)=0, \quad -1<x<1, \quad f(-1)=e, \quad f(1)=2/e.$$

If ε small, then discontinuity near $x=0$ (ex. $\varepsilon = 0.0001$)



Example of ODE

How to find the poles? $Lu = s$, $u(-1) = \alpha$, $u(1) = \beta$

- For ε small, solution near $x = 0$ behaves like $\frac{1}{2}\mathrm{erf}\left(\frac{2}{\sqrt{2\varepsilon}}\right) + 1.5 \approx 0.5\,\mathrm{sign}\,(x)$.
- Approximate this by a Padé approximant and take its poles (= complex poles very close to the origin).
  Take additional poles at ∞.
- Nodes $= \{x_k\}_0^N =$ zeros of Chebyshev ORF and $\{-1, 1\}$.
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  $L\tilde{u}(x_i) = \sum_{k=0}^{N} \hat{u}_k [L\phi_k](x_i) = s(x_i)$, $i = 1, \ldots, N-1$
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- For ε small, solution near $x = 0$ behaves like $\frac{1}{2}\mathrm{erf}\,(\frac{2}{\sqrt{2\varepsilon}}) + 1.5 \approx 0.5\,\mathrm{sign}\,(x)$.
- Approximate this by a Padé approximant and take its poles (= complex poles very close to the origin).
  Take additional poles at ∞.
- Nodes $= \{x_k\}_0^N =$ zeros of Chebyshev ORF and $\{-1, 1\}$.
- Solve interpolation conditions
  $L\tilde{u}(x_i) = \sum_{k=0}^{N} \hat{u}_k [L\phi_k](x_i) = s(x_i)$, $i = 1, \ldots, N-1$
  $\tilde{u}(-1) = \alpha, \quad \tilde{u}(1) = \beta$

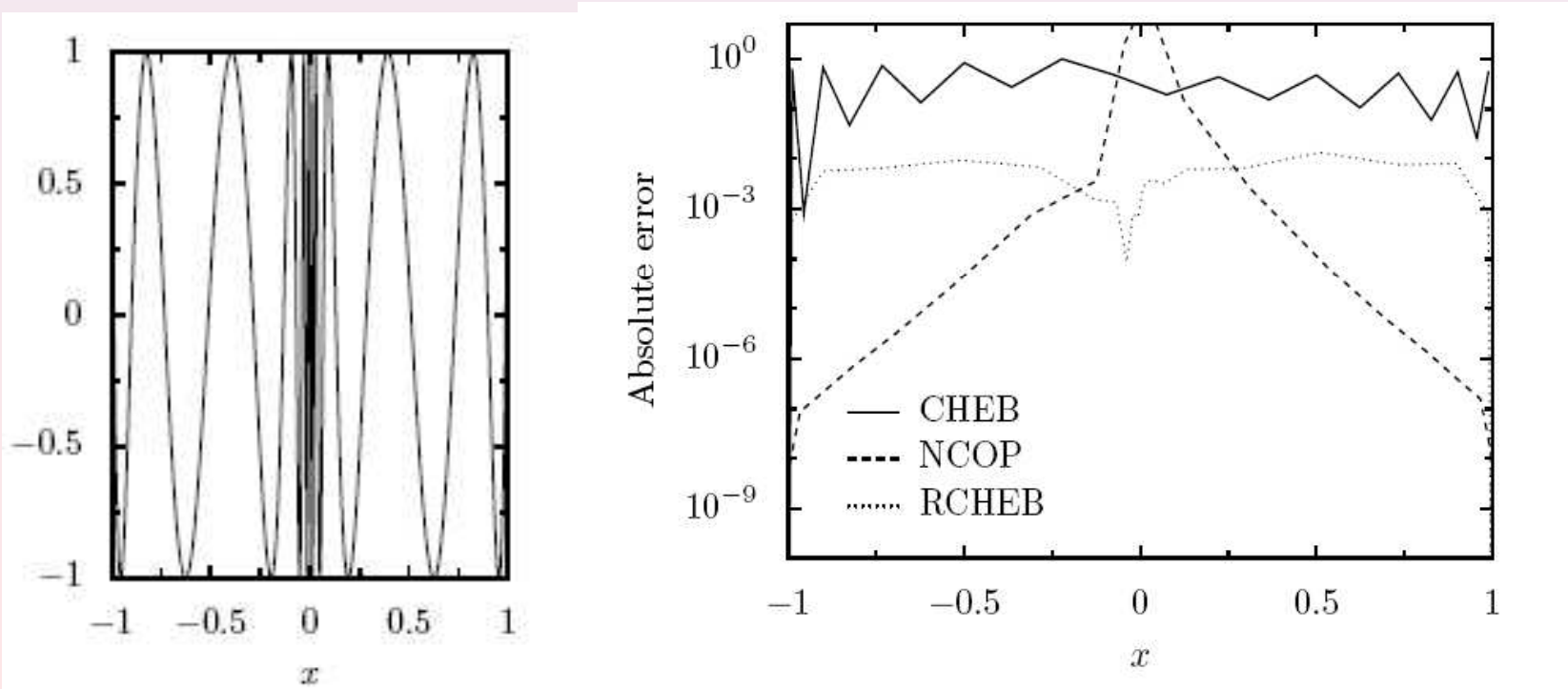
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Example of ODE

$N = 20$, 10 finite poles. Absolute error.
CHEB= Cheb OP, NCOP= Cheb OP 4 rational weight, RCHEB= Cheb ORF



Moment matrices

$E_n(z)^T = [e_0, e_1, \ldots, e_n]$ basis for $\mathcal{L}_n$
with moment matrix $M_n = [\langle e_i, e_j \rangle]$
Moment matrices are often structured (Toeplitz, Hankel,...)

$$\begin{aligned} k_n(z,w) &= \frac{-1}{\det M_n} \det \begin{bmatrix} M_n & E_m(z) \\ E_n(w)^H & 0 \end{bmatrix} \\ &= E_n(w)^H M_n^{-1} E_n(z) \quad \text{(Schur complement)} \end{aligned}$$

$\therefore$ recurrence for coef-vectors $\phi_k(z) = \mathbf{b}_k E_k(z)$
= fast algorithms for triangular factorization/inversion of M_n
$\therefore$ CD-relations = inversion formulas expressing M_n^{-1}.

ORF scalar case

- Given points $\{z_i\}_{i=1}^N \subset \mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$.
- Corresponding positive weights $\{w_i^2\}_{i=1}^N$.
- inner product $\langle f, g \rangle = \sum_{k=1}^N w_i^2 f(z_i)\overline{g(z_i)}$.
- Predefined poles $\{\alpha_k\}_{k=1}^N \subset \mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$.
- Nested spaces $\mathcal{L}_{n-1} \subset \mathcal{L}_n$:
  $\mathcal{L}_n = \{p_n(z)/\prod_{i=1}^n (z - \alpha_i) : p_n \in \Pi_n\}$
- ORF: $\phi_n \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$, $\phi_n \perp \mathcal{L}_{n-1}$
- This defines $\{\phi_n\}_{n=1}^N$

ORF scalar case

Lemma Set

$$\Phi(z) = [\phi_1(z), \phi_2(z), \ldots, \phi_N(z)],$$
$$\mathbf{A} = \mathrm{diag}(\alpha_1, \alpha_2, \ldots, \alpha_N),$$

Then there exists $\mathbf{H}$ = upper Hessenberg, with positive lower triangular elements such that

$$\Phi(z) = \Phi(z)(z\mathbf{I} - \mathbf{A})\mathbf{H}.$$

ORF scalar case

Theorem Set

$$\begin{aligned}
&\Phi(z) = [\phi_1(z), \phi_2(z), \ldots, \phi_N(z)],\\
&\mathbf{\Phi}_{i,j} = \phi_j(z_i),\\
&\mathbf{A} = \mathrm{diag}(\alpha_1, \alpha_2, \ldots, \alpha_N),\\
&\mathbf{Z} = \mathrm{diag}(z_1, z_2, \ldots, z_N),\\
&\mathbf{W} = \mathrm{diag}(w_1, w_2, \ldots, w_N),\\
&\mathbf{Q} = \mathbf{W}\mathbf{\Phi},
\end{aligned}$$

Then with $\mathbf{H}$ as before

$$\mathbf{Q} = (\mathbf{Z}\mathbf{Q} - \mathbf{Q}\mathbf{A})\mathbf{H}.$$

Inverse Eigenvalue Problem

$$\mathbf{Q} = (\mathbf{ZQ} - \mathbf{QA})\mathbf{H} \Rightarrow \mathbf{H}^{-1} = \mathbf{Q}^H\mathbf{ZQ} - \mathbf{A}$$

Hence setting $\mathbf{S} = \mathbf{H}^{-1}$, and fixing $\mathbf{Q}$ completely by letting $\mathbf{n}^H = [w_1\phi_1(z_1), \ldots, w_N\phi_1(z_N)]$, $\mathbf{n}^H\mathbf{Q} = [\|\mathbf{n}\|, 0, \ldots 0] =: \mathbf{n}_1^H$, (Normalisation = orthogonality w.r.t. first ORF) plus

$$\mathbf{Q}^H\mathbf{ZQ} = \mathbf{S} + \mathbf{A}$$

an inverse eigenvalue problem.
If all $\alpha_i = 0$

$$\mathbf{Q}^H\mathbf{ZQ} = \mathbf{S} \quad \text{or} \quad \mathbf{Q}^H\mathbf{Z}^{-1}\mathbf{Q} = \mathbf{H}$$

Semiseparable **S**

Because $\mathbf{H}$ is upper Hessenberg, $\mathbf{S} = \mathbf{H}^{-1}$ is lower semiseparable.
I.e. all submatrices of the lower triangular part of $\mathbf{S}$ (including the diagonal) have rank 1 at most.
Because $\mathbf{S} + \mathbf{A} = \mathbf{Q}^H \mathbf{Z} \mathbf{Q}$ is unitary, $\mathbf{S}$ is also upper semiseparable.

System theoretic applications

Want to find

$$\min \sum_{k=1}^{N} w_k^2 \left| y_k - \frac{p_N(z_k)}{q_N(z_k)} \right|^2$$

first approach:

$$\min \sum_{k=1}^{N} \left[\frac{w_k}{q_N(z_k)} \right]^2 \left| [y_k, -1] \begin{bmatrix} q_N(z_k) \\ p_N(z_k) \end{bmatrix} \right|^2 = \min \sum_{k=1}^{N} \phi_N(z_k)^H W_k \phi_N(z_k)$$

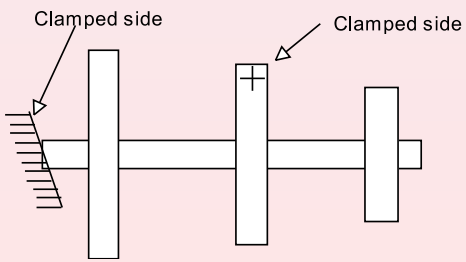
$$\phi_N(z) = \begin{bmatrix} q_N(z) \\ p_N(z) \end{bmatrix}, \quad W_k = \begin{bmatrix} y_k \\ -1 \end{bmatrix} \left[\frac{w_k}{q_N(z_k)} \right]^2 [y_k, -1].$$

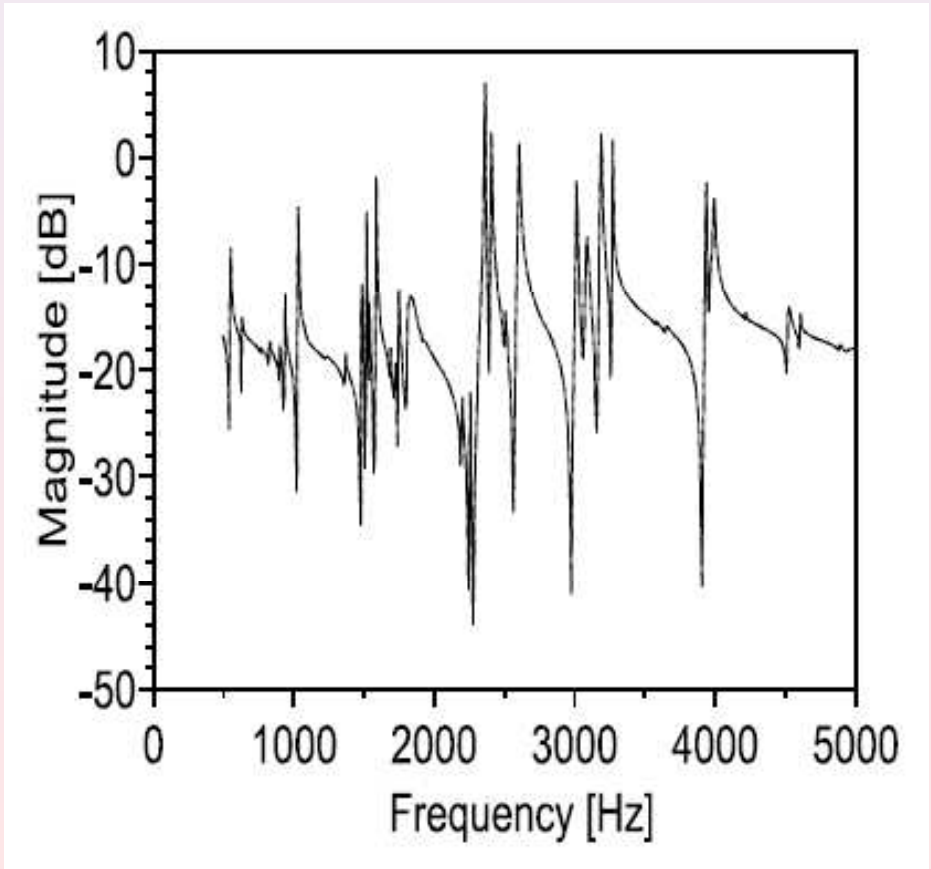
$\Rightarrow$ vector orthogonal polynomial ϕ_N

$\Rightarrow$ block version of polynomial IEP

Example: Vibrating system

Transfer functions can be pretty complicated (degree 120)





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second approach: given estimates of α_k

$$\frac{p_N(z)}{q_N(z)} = \sum_{k=1}^{N} a_k \phi_k(z), \quad \phi_k \in \mathcal{L}_k \setminus \mathcal{L}_{k-1}.$$

Linear problem. Needs ORF with $\alpha_k \neq 0$.
For real problems: we have pairs $(z_k, \overline{z}_k)$ and $(\alpha_k, \overline{\alpha}_k)$

Can we then do $\mathbf{Q}^H[\mathbf{n}|\mathbf{Z}] \left[\begin{array}{c|c} 1 & \\ \hline & \mathbf{Q} \end{array}\right] = [\mathbf{n}_1|\mathbf{S}+\mathbf{A}]$ in real arithmetic?

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Real ORF = RORF

Need to introduce complex conjugate pairs simultaneously.
Should result in numerator and denominator having real coefs.
Assume all $\alpha_k \neq 0$ then with $\pi_k(z) = \prod_{i=1}^{k}(z-\alpha_i)(z-\overline{\alpha}_i)$

$$B_k = \left\{ \frac{1}{\pi_k(z)(z-\alpha_{k+1})}, \frac{1}{\pi_{k+1}(z)} \right\} \text{ and } \tilde{B}_k = \left\{ \frac{1}{\pi_{k+1}(z)}, \frac{z}{\pi_{k+1}(z)} \right\}$$

span the same space.

$$\begin{aligned}
\mathcal{L}_N = \mathcal{L}_{2n} &= \operatorname{span}\{B_1, \ldots, B_n\} \\
&= \operatorname{span}\left\{\phi_1, \tilde{\phi}_1, \ldots, \phi_n, \tilde{\phi}_n\right\} \quad (C)ORF \\
&= \operatorname{span}\left\{\tilde{B}_1, \ldots, \tilde{B}_n\right\} \\
&= \operatorname{span}\left\{\psi_1, \tilde{\psi}_1, \ldots, \psi_n, \tilde{\psi}_n\right\} \quad RORF
\end{aligned}$$

Computation of eigenvalues, solution of linear systems

- A is a Hilbert space operator (e.g. $A \in \mathbb{R}^{N \times N}$)
- Krylov subspace
  $\mathcal{K}_{n+1}(A, v) = \text{span}\{v_0, \ldots, v_n\}, \quad v_k = A^k v, \quad v \in \mathbb{R}^N$
- project problem on low dimensional subspace $\mathcal{K}_{n+1}(A, v)$
- need orthogonal basis for $\mathcal{K}_{n+1}(A, v)$: $\{q_0, \ldots, q_n\}$,
  $q_k = \phi_k(A)v$, ϕ_k a polynomial of degree k
- If A is symmetric then:
  $q_k^T q_l = \delta_{kl} \Leftrightarrow \langle \phi_k, \phi_l \rangle = \delta_{kl}$, with inner product defined as
  $\langle \phi_k, \phi_l \rangle = L(\phi_k \phi_l)$ and the linear functional L is defined by
  the moments $L(z^k) = m_k = v^T A^k v$.
- This is classical Lanczos (3-term recurrence relation for OPS)

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eigenvalues

- power method $\Rightarrow$ q_k converges to eigenvector for largest eigenvalue
- if eigenvalue near α is required: iterate with $B = (A - \alpha I)^{-1}$
- Rational Krylov (Ruhe) different α_k in every step: $v_k = (A - \alpha_k I)^{-1} v_{k-1}$
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Model reduction

$$\begin{cases} C\frac{dx}{dt} = -Gx(t) + rw(t) \\ y(t) = l^H x(t) \end{cases} \rightarrow \mathcal{L} \rightarrow \begin{cases} sC\hat{x}(s) = -G\hat{x}(s) + r\hat{w}(t) \\ \hat{y}(s) = l^H \hat{x}(s) \end{cases}$$

$$\Rightarrow F(s) = \frac{\hat{y}(s)}{\hat{w}(s)} = l^H(G + sC)^{-1}r$$

Lanczos: biorthogonalization of $\mathcal{K}_{n+1}(A, v)$ and $\mathcal{K}_{n+1}(A^H, u)$
$u_0 = l$, $v_0 = (G + s_0 C)^{-1} r$, $A = -(G + s_0 C)^{-1} C$
$\Rightarrow U_n^H V_n = D_n$ and tridiagonal matrices (OP orthogonality) T_n, $\tilde{T}_n$
Large $A \rightarrow$ small T: $U_n^H A V_n = D_n T_n$ etc.
Large system projected onto a small Krylow space. spectrum of T are Ritz values $\approx$ spectrum of A

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Lanczos: biorthogonalization of $\mathcal{K}_{n+1}(A, v)$ and $\mathcal{K}_{n+1}(A^H, u)$

$u_0 = l$, $v_0 = (G + s_0 C)^{-1} r$, $A = -(G + s_0 C)^{-1} C$

$\Rightarrow U_n^H V_n = D_n$ and tridiagonal matrices (OP orthogonality) T_n, $\tilde{T}_n$

Large $A \rightarrow$ small T: $U_n^H A V_n = D_n T_n$ etc.

Large system projected onto a small Krylow space. spectrum of T are Ritz values $\approx$ spectrum of A

Model reduction

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$F_n(s) = (u_0^H v_0)(e_1^H (I - \theta T_n)^{-1} e_1), \quad \theta = s - s_0$
is an (n/n) Padé approximant for $F(s)$ at the point s_0.
The moments $u_0^H A^k v_0$ are never computed!
Denominators of PA are (formal) OP.
Can also with only 1 Krylov space.
Then tridiagonal matrices replaced by a Hessenberg matrix.
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Second order system (vibration systems)

Solve $(K + \omega C - \omega^2 M)x = f$ for many ω with K, C, M large and sparse.

(to approximate transfer function $F(\omega) = I^H(K + \omega C - \omega^2 M)^{-1} f$)

A rational approximation to $x(\omega)$ has poles that are eigenvalues of a quadratic eigenvalue problem.

Second order Krylov space spanned by columns of orthogonal Q_n.

Project the problem onto this smaller space.

A Padé approximant for $x(\omega)$ will approximate the eigen modes of the system.

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Gaussian quadrature

- compute $\int_a^b f(x)w(x)dx$ by gaussian quadrature $\sum_{k=1}^n \lambda_k f(\xi_k)$
- exact for all f, polynomials of degree $2n-1$ if ξ_k are the n zeros of the nth orthogonal polynomial for weight $w(x)$ on $[a,b]$
- the $\lambda_k = 1/\sum_{j=0}^{n-1} |\phi_j(\xi_k)|^2$ are the Christoffel numbers
- but for a function of the form $f(x) = p_n(x)/\prod_{j=1}^{n/2}(x^2+a_j^2)$ it would be better to be exact in spaces of rational functions
- so take ξ_k to be the zeros of the nth orthogonal rational function for space of rational functions whose poles are (near) the poles of f
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