Discrete orthogonal polynomials and superlinear convergence of Krylov subspace methods in numerical linear algebra

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OPSF summer school, Madrid, 8-18 July 2004

Menu

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- Rate of convergence of Krylov subspace methods and Ritz values
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- Motivation, link to discrete orthogonal polynomials
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- Further examples, Applications from PDE

Menu

- Motivation, link to discrete orthogonal polynomials §1.1
- Definition of Krylov subspace methods, polynomial language §1.2, 1.3, 1.4
- Logarithmic potential theory (with constraint) §2.1, 2.2, talk of AMF
- Asymptotics of discrete orthogonal polynomials §2.3
- Rate of convergence of Krylov subspace methods and Ritz values §3.1, 3.2
- Further examples, Applications from PDE §3.3, 3.4

Motivation

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- Asymptotics of discrete orthogonal polynomials
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A (very) simple example

Consider the system $Ax = b$ with

$$A = \text{diag}(1, 2, ..., N), \quad b = (1, ..., 1)^t / \sqrt{N},$$

and the discrete scalar product (of discrete Chebyshev polynomials)

$$\prec P, Q \succ = \sum_{j=1}^{N} \frac{1}{N} \overline{P(j)}\, Q(j)$$

with orthonormal polynomials p_k (that is, $\prec p_j, p_k \succ = \delta_{j,k}$ for $j, k < N$), then for the nth iterate x_n^{CG} of CG (with $x_0^{CG} = 0$) there holds

$$b - Ax_n^{CG} = A(x - x_n^{CG}) = \frac{p_n(A)b}{p_n(0)},$$

CG error for the (very) simple example

Write $\Lambda(A)$ for the spectrum of A, and let the $L_2(\Lambda(A))$-norm be induced by the above scalar product.

For the relative error of CG in energy norm ($||c||_A := \sqrt{c^* A c}$) one has

$$\begin{aligned}
\frac{||x_n^{CG} - x||_A}{||x_0^{CG} - x||_A} &= \frac{1}{|p_n(0)|} \\
&= \min_{\deg P \leqslant n} \frac{||P/\sqrt{x}||_{L_2(\Lambda(A))}}{|P(0)|\,||1/\sqrt{x}||_{L_2(\Lambda(A))}} \\
&\leqslant \min_{\deg P \leqslant n} \frac{||P||_{L_\infty(\Lambda(A))}}{|P(0)|} \\
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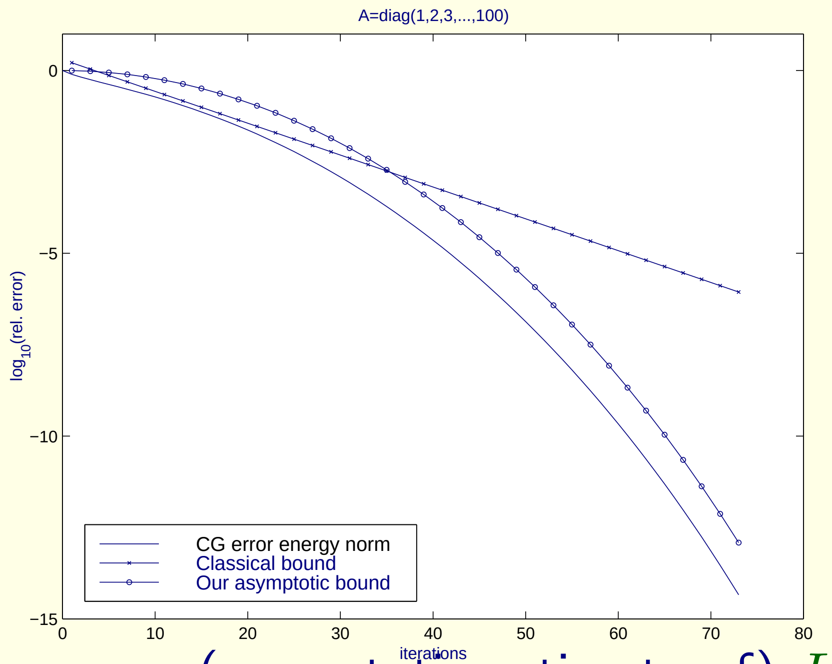
The different bounds

$A = \text{diag}(1, 2, \ldots, 100)$, random solution x, initial residual $r_0^{CG} = (1, ..., 1)^t$.



The CG error curve versus (asymptotic estimate of) $L_\infty(\Lambda(A))$ bound versus (classical) $L_\infty(\text{conv}(\Lambda(A)))$ bound:

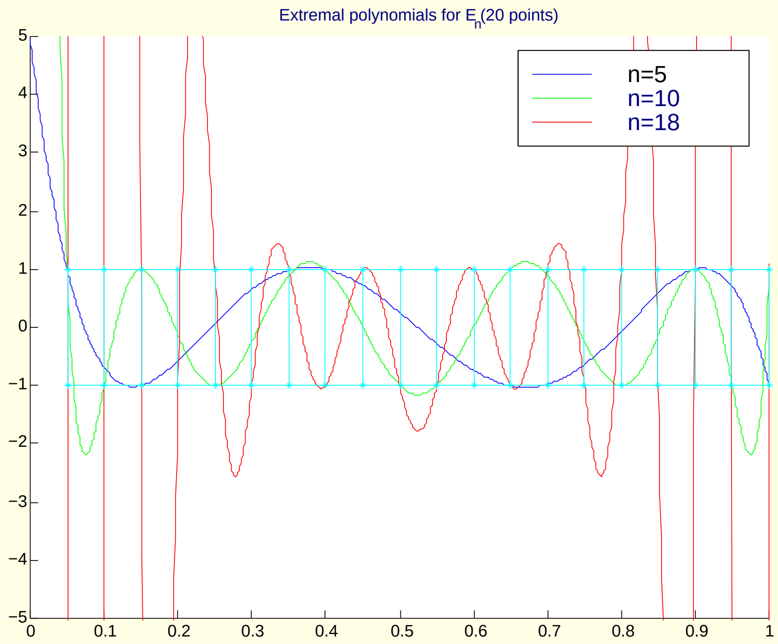
$$2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^n, \qquad \kappa = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}.$$

How to proceed?

- Asymptotics of discrete orthogonal polynomials?
  - $\ominus$ different from Szegő theory/classical nth root asymptotics
  - $\ominus$ we need to know precisely $\Lambda(A)$ (= finite (!) support)
  - $\ominus$ we need to know eigencomponents of starting residual (= weights)
  - $\oplus$ theory of Rakhmanov ('96) and Dragnev & Saff ('97) and ...
- Solve (approximately) the discrete L_∞ extremal problem?
  - $\oplus$ "worst case" bound for worst starting residual
  - $\oplus$ theory of Rakhmanov ('96) and Dragnev & Saff ('97) and ...
  - $\oplus$ simpler... (?!)

We have to find a polynomial large at zero and small on a discrete set.

Small on discrete sets



A polynomial small on $N = 20$ equidistant points is small in convex hull for degree $n = 5$, but no longer for $n = 10$ or $n = 18$.

Conclusion: We have to take into account the "fine structure" of $\Lambda(A)$.

What we've learned so far

Not so much (-; but don't worry, we will see everything again in greater detail.

Well, maybe one point: depending on the distribution of the elements, a polynomial being small on a discrete set is not necessarily small in the convex hull of this set, at least for larger degrees.

And, there seems to be some link between OP and linear algebra. But this you knew before?

Krylov subspace methods

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Definition Krylov subspace methods I

In this talk: $A = A^*$, of size $N \times N$.

- Solve systems of linear equations $Ax = b$,
  - Conjugate gradients ($A \geqslant 0$)
  - Lanczos
  - MinRes/GMRES
- Approach (certain) eigenvalues of A by Ritz values

Assumption: matvec product easy (A large, sparse)

Assumption for our analysis: rounding errors neglected

Construct sequence x_0 (given), $x_1, x_2, \ldots$ converging to $A^{-1}b$
with residuals $r_n = r(x_n) := b - Ax_n$

Definition Krylov subspace methods II

Krylov subspace:

$\mathcal{K}_n(A,c) = \text{span}\{c, Ac, A^2c, ..., A^{n-1}c\} = \{p(A)c : p$ a polynomial of degree $\leqslant n-1\}$.

Here $x_n \in x_0 + \mathcal{K}_{n-1}(A, r_0)$, and hence for some polynomial q_n of degree n

$$r_n = \frac{q_n(A) r_0}{q_n(0)}.$$

- Conjugate gradients: $x_n^{CG} = \arg\min\{||r(x)||_{A^{-1}} : x \in x_0 + \mathcal{K}_n(A, r_0)\}$
- MinRes/GMRES: $x_n^{GMRES} = \min\{||r(x)|| : x \in x_0 + \mathcal{K}_n(A, r_0)\}$
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The scalar product

Here $A = A^*$ and thus $A = VDV^*$, V unitary, $D = \text{diag}(\lambda_1, ..., \lambda_N)$.

Let $V^* r_0 =: \beta = (\beta_1, \beta_2, ..., \beta_N)$, and define for polynomials P, Q the scalar product

$$\prec P, Q \succ = (P(A) r_0)^* Q(A) r_0 = (VP(D)V^* r_0)^* VQ(D)V^* r_0 = \sum_j |\beta_j|^2 \, \overline{P(\lambda_j)} \, Q(\lambda_j)$$

(more complicated if $A \neq A^*$, see §1.3, Example 1.3.8). Define $N' \leqslant N$ the number of distinct λ_j with non-zero β_j, then we can define orthonormal polynomials

$$j = 0, ..., N'-1: \qquad p_j(z) = k_j z^j + \text{ lower powers}, \qquad k_j > 0,$$
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How to express x_n^L, x_n^{GMRES}, x_n^{CG} in terms of p_n?

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How to express x_n^L, x_n^{GMRES}, x_n^{CG} in terms of p_n?

Arnoldi basis

By construction, the vectors $v_{n+1} := p_n(A) r_0$ satisfy

$$1 \leqslant n \leqslant N' : \qquad v_n \in \mathcal{K}_n(A, r_0), \qquad v_n \perp \mathcal{K}_{n-1}(A, r_0),$$
$$v_{N'+1} = 0,$$

and hence (c.f. 1.2.2)

$$\text{for } n \leqslant N' : \qquad \dim \mathcal{K}_n(A, r_0) = n, \quad \text{with ONB } v_1, v_2, ..., v_n,$$
$$\text{for } n \geqslant N' : \qquad \dim \mathcal{K}_n(A, r_0) = N', \quad \text{with ONB } v_1, v_2, ..., v_{N'}.$$

Idea: express r_n^L, r_n^{GMRES}, r_n^{CG} in terms of the Arnoldi basis!

FOM = sym. Lanczos (if $A = A^*$)

r_n^L is in $\mathcal{K}_{n+1}(A, r_0)$ and $\perp$ to $\mathcal{K}_n(A, r_0)$, like v_{n+1}, c.f. 1.3.4.

Thus x_n^L exists iff $p_n(0) \neq 0$ ("breakdown"), and then

$$r_n^L = \frac{p_n(A) r_0}{p_n(0)} = \frac{1}{p_n(0)} v_{n+1}, \qquad ||r_n^L|| = \frac{1}{|p_n(0)|}.$$

GMRES/MINRES

By definition of GMRES

$$||r_n^{GMRES}||^2 = \min_{\deg P \leqslant n} \frac{\prec P, P \succ}{|P(0)|^2} = \frac{1}{K_{n,2}(0,0)},$$

with the Szegő function

$$K_{n,2}(x,y) = \sum_{j=0}^{n} \overline{p_j(x)} p_j(y),$$

and the minimum is attained for $P(z) = K_{n,2}(0,z)$.

Hence (c.f. 1.3.6)

$$r_n^{GMRES} = \frac{K_{n,2}(0,A) r_0}{K_{n,2}(0,0)} = \frac{1}{K_{n,2}(0,0)} \sum_{j=0}^{n} \overline{p_j(0)}\, v_{j+1}.$$

CG (for $A = A^*$, $A > 0$)

With the same argument as for GMRES/MINRES

$$||r_n^{CG}||^2_{A^{-1}} = \frac{1}{K^{\#}_{n,2}(0,0)}, \qquad , \qquad r_n^{CG} = \frac{K^{\#}_{n,2}(0,A)r_0}{K^{\#}_{n,2}(0,0)},$$

with the Szegő function $K^{\#}_{n,2}(x,y)$ constructed for the modified scalar product

$$\prec P, Q \succ^{\#} = \prec P, Q/z \succ .$$

From Christoffel-Darboux: $K^{\#}_{n,2}(0,z)$ is proportional to $p_n(z)$.

Hence $p_n(0) \neq 0$, and (c.f. 1.4.2)

$$r_n^{CG} = r_n^L = \frac{p_n(A)r_0}{p_n(0)} = \frac{1}{p_n(0)}\, v_{n+1}, \qquad ||r_n^{CG}|| = \frac{1}{|p_n(0)|}.$$

See 1.4.1(g), 1.4.2 for a link between CG and Padé approximants of the rational function $z \mapsto r_0^*(zI - A)^{-1} r_0$.

Corollary: L_∞ bounds

Let

$$E_n(z,S) := \min_{p\in P_n} \max_{\lambda\in S} \frac{|p(\lambda)|}{|p(z)|}$$

then $K_{0,2}(0,0)/K_{n,2}(0,0) \leqslant E_n(0,\Lambda(A))^2$, and hence

$$\frac{||r_n^{GMRES}||}{||r_0^{GMRES}||} \leqslant E_n(0,\Lambda(A)), \qquad \frac{||r_n^{CG}||_{A^{-1}}}{||r_0^{CG}||_{A^{-1}}} \leqslant E_n(0,\Lambda(A)).$$

Remarks:

- $E_n(z,S)$ is decreasing in n and increasing in S,
- for $a \neq 0$: $E_n(z,aS) = E_n(z/a,S) = E_n(0,S-z/a)$,
- the extremal polynomial for $E_n(z,[-1,1])$, $z \in \mathbb{R}\setminus[-1,1]$ is the Chebyshev polynomial of the first kind, c.f. 1.4.6, 1.4.7
  $\Longrightarrow$ classical CG bound in terms of condition number.

Jacobi matrices

Define the Jacobi matrix (upper Hessenberg if $A \neq A^*$, c.f. 1.2.5, 1.3.2)

$$J_n := \Big[\prec p_j, z p_k \succ \Big]_{j,k} = \begin{bmatrix} b_0 & a_0 & 0 & \cdots & \cdots & 0 \\ a_0 & b_1 & a_1 & 0 & \cdots & 0 \\ 0 & a_1 & b_2 & a_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a_{n-3} & b_{n-2} & a_{n-2} \\ 0 & \cdots & \cdots & 0 & a_{n-2} & b_{n-1} \end{bmatrix},$$

then

$$z(p_0, p_1, ..., p_{n-1})(z) = (p_0, p_1, ..., p_{n-1})(z) J_n + a_{n-1} p_n(z)(0, ..., 0, 1).$$

Note: eigenvalues of J_n are zeros of OP p_n!

Computing Jacobi matrix through Arnoldi basis

Writing $V_n := (v_1, ..., v_n) \in \mathbb{C}^{N \times n}$, we get

$$AV_n = V_n J_n + a_{n-1}(0, ..., 0, v_{n+1}).$$

- Recursive way of computing v_n, J_n,
- three term recurrence for the v_n (in case $A = A^*$).

Ritz values

The eigenvalues of the orthogonal projection $J_n = V_n^* A V_n$ are called the nth Ritz values of A.

"Lucky" breakdown $AV_{N'} = V_{N'} J_{N'}$ (i.e., the columns of $V_{N'}$ form an A-invariant subspace), and $N' \ll N$.

Interlacing/separation: write $\lambda_1 \leqslant \lambda_2 \leqslant ... \leqslant \lambda_N$ for the spectrum of A, $x_{1,n} < x_{2,n} < ... < x_{n,n}$ for the nth Ritz values, then

$$x_{j,n+1} < x_{j,n} < x_{j+1,n+1}$$

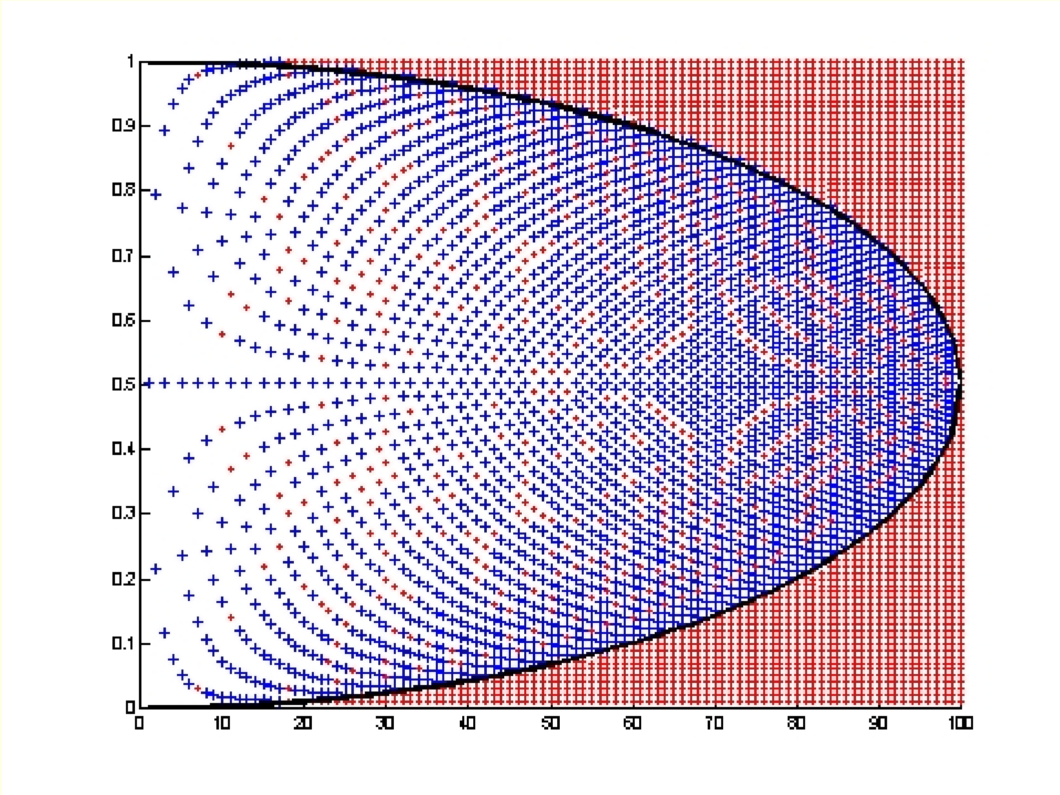
$$\lambda_1 \leqslant x_{j,n} \leqslant \lambda_N$$

$$\forall \kappa < n \, \exists k : \qquad x_{\kappa,n} \leqslant \lambda_k \leqslant x_{\kappa+1,n}.$$

Approaching eigenvalues by Ritz values? Which ones?

An example for convergence of Ritz values

100 equidistant eigenvalues in $[0, 1]$. We draw vertically the nth Ritz values for $n = 1, 2, ..., 100$. A Ritz value is red if closer than 10^{-3} to some eigenvalue.



An example for convergence of Ritz values (continued)

Observations:

- In most of the cases (up to some "accidents"): once there is a Ritz value close to an eigenvalue λ_j, this λ_j is well approximated also for larger n.
  We say that a Ritz value "converged".
  More precisely, one can show that that for $x \in \Lambda(J_n)$, $y \in \Lambda(J_{n+1})$

  $$\max\{\text{dist}(x, \Lambda(A)), \text{dist}(y, \Lambda(A))\} \leqslant 2\sqrt{|x-y|\,(\lambda_{\max}(A) - \lambda_{\min}(A))}.$$

- Ritz values closer to $0, 1$ seem to converge faster.

- Some particular black line (half circle) seems to separate the converged and the non-converged Ritz values.

Trefethen & Bau '97, Kuijlaars '00, BB

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Ritz and CG/GMRES

Linear algebra interpretation:

Eigenvalues matched by Ritz values should no longer be taken into account for CG convergence history

$\Longrightarrow$ decreasing "marginal condition number" ?!

Kaniel-Page-Saad estimate for extremal eigenvalues

$$x_{1,n} - \lambda_1 \leqslant \frac{\lambda_N - \lambda_1}{T_{n-1}(1 + 2\frac{\lambda_2 - \lambda_1}{\lambda_N - \lambda_2})^2} \frac{1}{|\beta_1|^2} \sum_{j=2}^{N} |\beta_j|^2,$$

with T_n being the nth Chebyshev polynomial of the first kind.

Right-hand side small if λ_1 "far" from rest of spectrum, $|\beta_1|$ not too small.

New bounds also for inner eigenvalues

If $\lambda_k \leqslant x_{1,n}$ then $x_{1,n} - \lambda_k$ equals

$$\min\left\{ \frac{\sum_{j \neq k} |\beta_j|^2 (\lambda_j - x_{1,n}) |q(\lambda_j)|^2}{|\beta_k|^2 |q(\lambda_k)|^2} : \deg q < n, q(\lambda_k) \neq 0 \right\}.$$

Here the minimum is attained for the polynomial $q(x) = p_n(x)/(x - x_{1,n})$.

If $\lambda_k \in [x_{1,n}, x_{n,n}]$, say, $x_{\kappa-1,n} \leqslant \lambda_k \leqslant x_{\kappa,n}$, then $(\lambda_k - x_{\kappa-1,n})(x_{\kappa,n} - \lambda_k)$ equals

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Idea of proof for this (second) bound

Step 1: Gaussian quadrature: if $\deg P \leqslant 2n-1$ then

$$\prec 1, P \succ = \sum_{j=1}^{n} \frac{P(x_{j,n})}{K_{n,2}(x_{j,n}, x_{j,n})}.$$

Step 2: positivity of a certain polynomial: let

$$P(z) = (z - x_{\kappa-1,n})(z - x_{\kappa,n})\, q(z)\, \overline{q(\overline{z})}, \qquad \deg q \leqslant n-2,$$

then $\prec 1, P \succ \geqslant 0$ (and $= 0$ for the given polynomial q).

Step 3: solve

$$\prec 1, P \succ = \sum_{j} |\beta_j|^2 \, P(\lambda_j) \geqslant 0$$

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If $\lambda_k \leqslant x_{1,n}$ then

$$x_{1,n} - \lambda_k \leqslant (\lambda_N - \lambda_1)\, E_{n-1}(\lambda_k, \Lambda(A) \setminus \{\lambda_k\})^2 \, \frac{1}{|\beta_1|^2} \sum_{j \neq k} |\beta_j|^2.$$

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What we've learned so far

- Lanczos, CG and GMRES residuals can be expressed in terms of discrete OP
- their error can be bounded in terms of "classical" discrete L_2 or L_∞ extremal problems
- Ritz values are just zeros of discrete OP, they should approach set of EV = support of measure of orthogonality
- the distance of an eigenvalue to the set of Ritz values can be bounded in terms of discrete L_2 or L_∞ extremal problems

Logarithmic potential theory with constraint

Basic definitions

$\mathcal{M}_t(\Sigma)$: set of Borel measures μ with support $\mathrm{supp}\,(\mu) \subset \Sigma$ (Σ compact) and mass $||\mu|| := \mu(\Sigma) = t$.

Logarithmic potential and the energy of a measure

$$U^\mu(z) = \int \log(\frac{1}{|x-z|})\,d\mu(x), \quad I(\mu) = \int\int \log(\frac{1}{|x-y|})\,d\mu(x)\,d\mu(y).$$

External field $Q \in \mathcal{C}(\Sigma)$: weighted energy $I^Q(\mu) = I(\mu) + 2\int Q\,d\mu$.

Why logarithmic potentials?

$$P(z) = \prod_{j=1}^{n}(z-z_j), \quad \nu_N(P) = \frac{1}{N}\sum_{j=1}^{n}\delta_{z_j} \quad \Longrightarrow \quad -\log(|P(z)|^{1/N}) = U^{\nu_N(P)}(z),$$

and discrete measures are dense in $\mathcal{M}_t(\Sigma)$.

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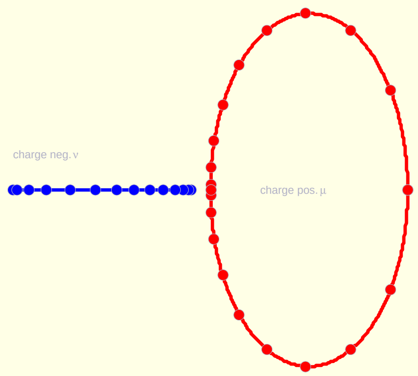
- μ: electric charge in $\mathbb{R}^2$ (or cylinder-symmetric in $\mathbb{R}^3$).
- $I(\mu)$ electric energy, U^μ electric potential of a positive charge μ.
- Minimize $I(\mu)$, $\mu \in \mathcal{M}_1(\Sigma)$: find electrostatic equilibrium of unit charge on conductor Σ (Faraday principle).
- Minimize $I^Q(\mu)$, $\mu \in \mathcal{M}_1(\Sigma)$: presence of an external force Q coming from, e.g., a negative/positive fixed charge on some isolator (problem of balayage).



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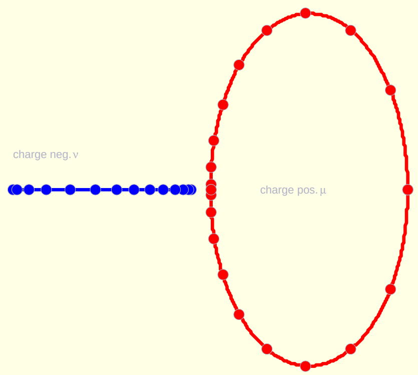

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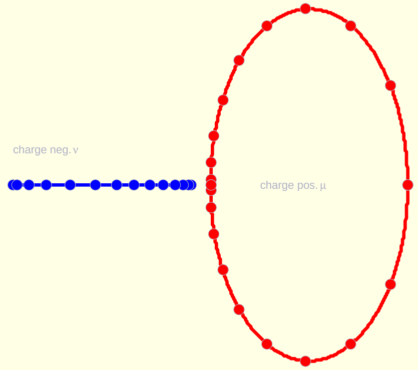

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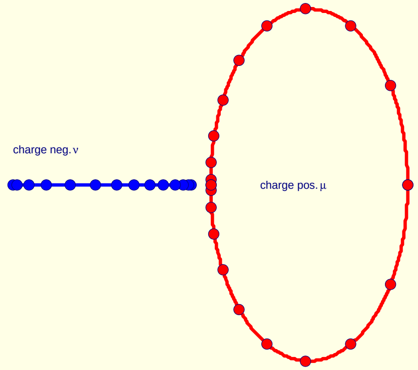

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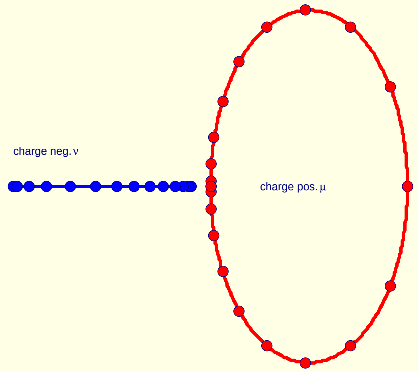

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Equilibrium with external field without constraint

Let Σ compact, "regular", $Q \in \mathcal{C}(\Sigma)$.

There exists a unique minimizer called $\mu_{t,Q,\Sigma}$ for the problem

$$\min\{I^Q(\mu) : \mu \in \mathcal{M}_t(\Sigma)\}.$$

Equilibrium conditions: with $\mu = \mu_{t,Q,\Sigma}$, $w = w_{t,Q,\Sigma}$ there holds

$$U^\mu(z) + Q(z) \geqslant w \qquad \text{for } z \in \Sigma, \text{ and} \qquad (1)$$

$$U^\mu(z) + Q(z) \leqslant w \qquad \text{for } z \in \operatorname{supp}(\mu). \qquad (2)$$

Conversely, if (1) and (2) for some measure $\mu \in \mathcal{M}_t(\Sigma)$ then $\mu = \mu_{t,Q,\Sigma}$.

- Green function ($Q = 0$):
  $g_\Sigma(z) = w_{t,0,\Sigma} - U^{\mu_{t,0,\Sigma}}(z) = \log(|z|) - \log(\operatorname{cap}(\Sigma)) + o(1)_{|z|\to\infty}$.
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Equilibrium conditions: with $\mu = \mu_{t,Q,\Sigma}$, $w = w_{t,Q,\Sigma}$ there holds

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- Green function ($Q = 0$):
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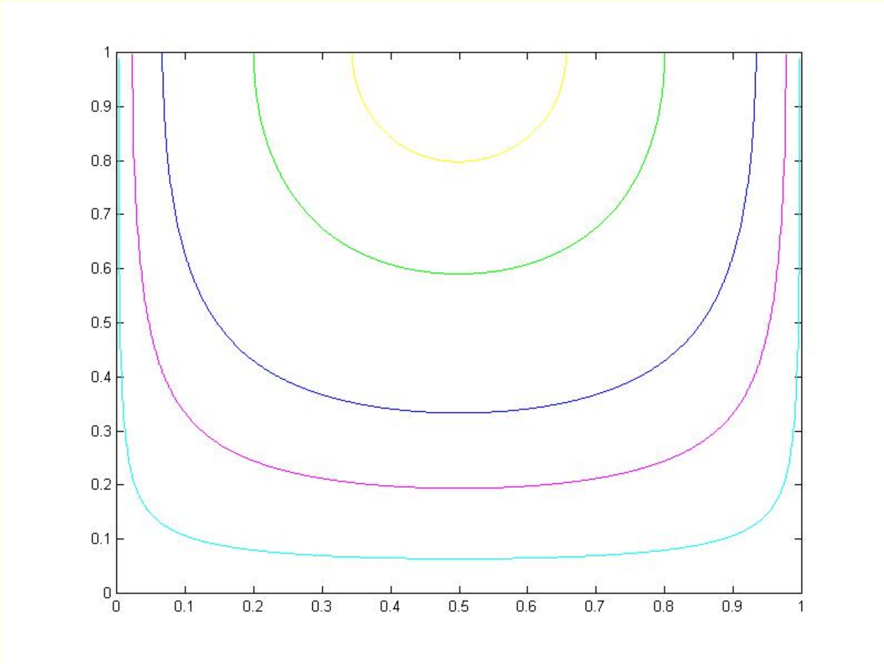
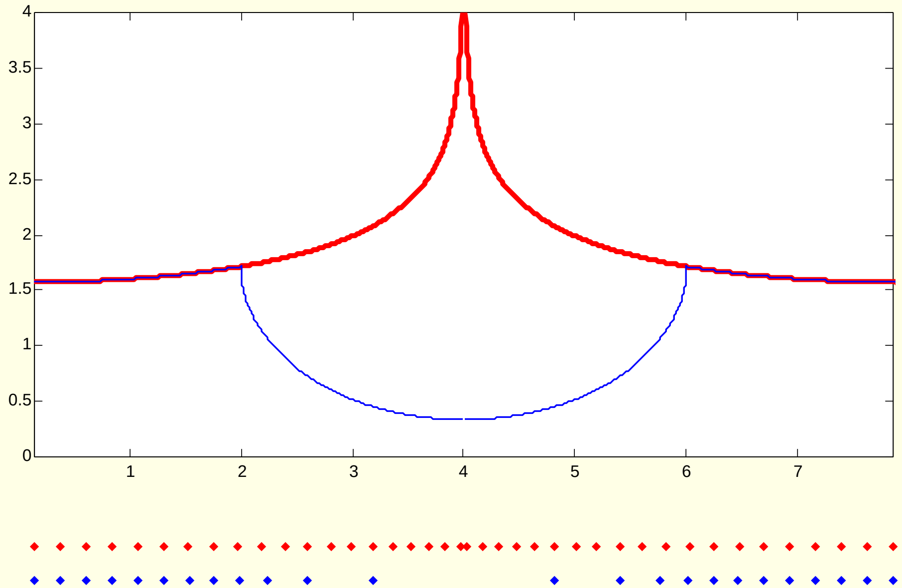
Constraint = maximum charge





On the left: density of equilibrium measure for $Q = 0$, $d\sigma = dx$ Lebesgue measure on $[0, 1]$ and $t = 0.95, 0.8, 0.5, 0.3, 0.1$.

Observations: $\mathrm{supp}\,(\mu_{t,0,\sigma}) = \mathrm{supp}\,(\sigma)$, $\mathrm{supp}\,(\sigma - \mu_{t,0,\sigma})$ decreases in t.

Idea of proof for the two theorems

Let $\mathcal{N} \subset \mathcal{M}_t(\Sigma)^*$ closed & convex, and consider $\min\{I^Q(\mu) : \mu \in \mathcal{N}\}$.

Step 1: existence of minimizer $\mu_{\mathcal{N}}$. Helly's principle and lower semi-continuity

$$\mu_n \xrightarrow{*} \mu \quad \Longrightarrow \quad \liminf_n I^Q(\mu_n) \geqslant I^Q(\mu).$$

Step 2: uniqueness of minimizer $\mu_{\mathcal{N}}$. The map $\mathcal{N} \ni \mu \mapsto I^Q(\mu)$ is strictly convex.

Step 3: minimizer $\Longrightarrow$ equilibrium. By convexity,

$$\forall \mu \in \mathcal{N} : \qquad \int [U^{\mu_{\mathcal{N}}} + Q]\, d\mu_{\mathcal{N}} \leqslant \int [U^{\mu_{\mathcal{N}}} + Q]\, d\mu. \tag{5}$$

Use also "Principle of domination" (c.f. 2.1.7).

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- Case with Q without σ (talk of AMF, work of Buyarov & Rakhmanov '99):

we have formulas for $\mu_{t,Q,\Sigma}$, Q once we know $\mathrm{supp}\,(\mu_{t,Q,\Sigma})$ for all t.

- Case with $Q = 0$ and integral formula for σ: if $S(t)$ decreasing sets in t then

$$\sigma(x) = \int_0^{||\sigma||} \omega_{S(t)}(x)\,dt \quad \Longrightarrow \quad w_{t,0,\sigma} - U^{\mu_{t,0,\sigma}}(z) = \int_0^t g_{S(\tau)}(z)\,d\tau,$$

where $\omega_S := \mu_{1,0,S}$ Robin equilibrium distribution, c.f. 2.1.1, 2.2.6, 2.2.7.

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What we've learned so far

- minimizing logarithmic energy means looking for electro-static equilibrium in plane
- even in presence of external field and/or an upper constraint, electro-static equilibrium is unique, and can be characterized by equilibrium conditions
- logarithmic potential theory is natural to describe nth root asymptotics of moduli of polynomials of degree n.
- solving (exactly) an equilibrium problem is in general difficult, often we get (systems of) integral equations for the endpoints of the supports
- there are some nice integral formulas for the equilibrium potential

Asymptotics of discrete orthogonal polynomials

- Motivation, link to discrete orthogonal polynomials
- Definition of Krylov subspace methods, polynomial language
- Logarithmic potential theory (with constraint)
- Asymptotics of discrete orthogonal polynomials
- Rate of convergence of Krylov subspace methods and Ritz values
- Further examples, Applications from PDE

Part 2 Part 3

Discrete Chebyshev, Meixner, Charlier, etc.

Consider ONP $p_{n,N}$ with respect to the discrete scalar product

$$\prec P, Q \succ = \sum_{z \in E_N} w_N(z)^2 \, \overline{P(z)} \, Q(z)$$

e.g., $E_N = \{0, 1, ..., N\}$, $w_N = 1$ (discrete Chebyshev) or $E_N = \{0, 1, 2, ...\}$, and $w_N(k)^2 = \frac{c^k (b)_k}{k!}$ (Meixner) or $w_N(k)^2 = \frac{c^k e^{-c}}{k!}$ (Charlier) or ...

- Question: $|p_{n,N}(N^\alpha z)|^{1/N} \to ?$ for $n, N \to \infty$, $n/N \to t > 0$?
- Answer: extremal problem with constraint and external field, c.f. Rakhmanov '96, Dragnev & Saff '97
- Further results: Kuijlaars & Van Assche '99, Kujlaars & Rakhmanov '98, BB '00a, Damelin & Saff '98?
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- Question: $|p_{n,N}(N^\alpha z)|^{1/N} \to ?$ for $n, N \to \infty$, $n/N \to t > 0$?
- Answer: extremal problem with constraint and external field, c.f. Rakhmanov '96, Dragnev & Saff '97
- Further results: Kuijlaars & Van Assche '99, Kujlaars & Rakhmanov '98, BB '00a, Damelin & Saff '98?
- Applications: Random matrices (Johansson '00), Continuum limit of Toda lattice (Deift & McLaughlin '00, ...), coding theory,...

Discrete Chebyshev, Meixner, Charlier, etc.

Consider ONP $p_{n,N}$ with respect to the discrete scalar product

$$\prec P, Q \succ = \sum_{z \in E_N} w_N(z)^2 \, \overline{P(z)} \, Q(z)$$

e.g., $E_N = \{0, 1, ..., N\}$, $w_N = 1$ (discrete Chebyshev) or $E_N = \{0, 1, 2, ...\}$, and $w_N(k)^2 = \frac{c^k (b)_k}{k!}$ (Meixner) or $w_N(k)^2 = \frac{c^k e^{-c}}{k!}$ (Charlier) or ...

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Thm 2.3.2: notation

Discrete L_p norm

$$||wQ||_{L_p(E_N)} = \left[\sum_{z\in E_N} w(z)^p\,|Q(z)|^p\right]^{1/p}, \qquad ||wQ||_{L_\infty(E_N)} = \sup_{z\in E_N} |w(z)Q(z)|.$$

Set counting measure

$$\nu_N(E_N) = \frac{1}{N}\sum_{z\in E_N}\delta_z.$$

Discrete energy

$$I_N(E_N) = \frac{1}{N^2}\sum_{x\in E_N}\sum_{y\in E_N, y\neq x}\log(\frac{1}{|x-y|}).$$

Lower semi-continuity:

$$\nu_N(E_N) \xrightarrow{*} \sigma \quad \Longrightarrow \quad \liminf_N I_N(E_N) \geqslant I(\sigma).$$

Thm 2.3.2 "light": Σ compact

Suppose that

(H1) $\forall N: \quad E_N \subset \Sigma$ with Σ compact

(H2) $\nu_N(E_N) \xrightarrow{*} \sigma$, with $U^\sigma \in \mathcal{C}(\Sigma)$,

(H3) $\limsup_N \sup_{z \in E_N} w_N(z)^{1/N}/e^{-Q(z)} \leqslant 1$, with $Q \in \mathcal{C}(\Sigma)$,

(H4) $\mathrm{supp}\,(\mu_{t,Q,\sigma}) \cap \mathrm{supp}\,(\sigma - \mu_{t,Q,\sigma}) \neq \emptyset$,

Then for all $z \notin \Sigma$

$$\limsup_{n,N\to\infty, n/N\to t} \left[\min_{\deg P \leqslant n} \frac{||w_N \cdot P||_{L_p(E_N)}}{|P(z)|} \right]^{1/N} \leqslant \exp(U^{\mu_{t,Q,\sigma}}(z) - w_{t,Q,\sigma}). \quad (6)$$

More generally, limit is true for all z with **(H6)**: $\limsup_N U^{\nu_N(E_N)}(z) \leqslant U^\sigma(z)$.

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Suppose that

$$\begin{array}{lll} \textbf{(H1)} & \forall N: \quad E_N \subset \Sigma & \text{with } \Sigma \text{ compact} \\ \textbf{(H2)} & \nu_N(E_N) \xrightarrow{*} \sigma, & \text{with } U^\sigma \in \mathcal{C}(\Sigma), \\ \textbf{(H3)} & \limsup_N \sup_{z \in E_N} w_N(z)^{1/N}/e^{-Q(z)} \leqslant 1, & \text{with } Q \in \mathcal{C}(\Sigma), \\ \textbf{(H4)} & \operatorname{supp}(\mu_{t,Q,\sigma}) \cap \operatorname{supp}(\sigma - \mu_{t,Q,\sigma}) \neq \emptyset, & \end{array}$$

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Then for all $z \notin \Sigma$

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More generally, limit is true for all z with **(H6)**: $\limsup_N U^{\nu_N(E_N)}(z) \leqslant U^\sigma(z)$.

Thm 2.3.2 "light": Σ compact (continued)

Suppose that

$$
\begin{array}{ll}
(\mathbf{H1}) & \forall N: \qquad E_N \subset \Sigma \qquad \text{with } \Sigma \text{ compact} \\
(\mathbf{H2}) & \nu_N(E_N) \xrightarrow{*} \sigma, \qquad \text{with } U^\sigma \in \mathcal{C}(\Sigma), \\
(\mathbf{H3})' & \limsup_N \sup_{z\in E_N} |e^{-Q(z)} - w_N(z)^{1/N}| = 0, \qquad \text{with } Q \in \mathcal{C}(\Sigma), \\
(\mathbf{H4}) & \operatorname{supp}(\mu_{t,Q,\sigma}) \cap \operatorname{supp}(\sigma - \mu_{t,Q,\sigma}) \neq \emptyset, \\
(\mathbf{H5}) & \limsup_N I_N(E_N) \leqslant I(\sigma).
\end{array}
$$

Then for all $z \notin \Sigma$

$$\lim_{n,N\to\infty, n/N\to t} \left[\min_{\deg P \leqslant n} \frac{||w_N \cdot P||_{L_p(E_N)}}{|P(z)|} \right]^{1/N} = \exp(U^{\mu_{t,Q,\sigma}}(z) - w_{t,Q,\sigma}). \quad (7)$$

More generally, limit is true for all z with **(H6)**: $\limsup_N U^{\nu_N(E_N)}(z) \leqslant U^\sigma(z)$.

Thm 2.3.2 for general Σ

More assumptions:

- $\Sigma, \mathrm{supp}\,(\sigma)$ no longer compact. We need $\forall K$ compact: $U^{\sigma|_K}$ continuous;
- add decay rate for $w_N(z)$ and for $Q(z)$ for large $|z|$;
- impose **(H3)**, **(H3)'** only on compacts;
- restrict E_N, σ to suitable open set in **(H5)**, **(H6)**.

Remark: Assumption **(H5)** conjectured by Rakhmanov.

He introduced the stronger separation condition

$$\liminf_{N\to\infty} \inf_{x,y\in E_N, x\neq y} N^\alpha \, |x-y| > 0 \qquad \text{for } \alpha = 1.$$

Idea of proof for Thm 2.3.2 for compact Σ

Step 1: L_p-norms are equivalent (up to power of N), thus proof for $p = \infty$ sufficient.

Step 2 (discretization of $\mu_{t,Q,\sigma}$): for $\epsilon > 0$, let

$$K_\epsilon = \{\lambda \in \Sigma : U^{\mu_{t,Q,\sigma}}(\lambda) + Q(\lambda) \leqslant w_{t,Q,\sigma} - \epsilon\},$$

and determine $E_N^* \subset E_N$ with

$$E_N^* \subset E_N, \qquad E_N^* \cap K_\epsilon = E_N \cap K_\epsilon, \qquad \nu_N(E_N^*) \xrightarrow{*} \mu_{t,Q,\sigma} \quad \text{for } N \to \infty.$$

Step 3: with P_N having set of zeros E_N^*:
$\limsup ||e^{-NQ} P_N||_{L_\infty(E_N)}^{1/N} \leqslant \exp(-w_{t,Q,\sigma} + \epsilon)$ by construction and principle of descent,
$\lim |P_N(z)|^{1/N} = \exp(-U^{\mu_{t,Q,\sigma}}(z))$ by **(H6)** and principle of descent.

Step 4: constrained Fekete points minimizing $I_N(E_N') + 2\int Q d\nu_N(E_N')$ in E_N.

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Example discrete Chebyshev polynomials

$w_N = 1 \Longrightarrow Q = 0$,
$E_N = \{1/N, 2/N, ..., N/N\} \Longrightarrow \mathrm{supp}\,(\sigma) = \Sigma = [0,1]$, and

$$\frac{d\sigma}{dx}(x) = 1 = \int_{\arg\sqrt{\ }>0} \frac{1}{\pi\sqrt{(1-t^2)/4-(x-1/2)^2}}\,dt.$$

Thus $S(t) = \mathrm{supp}\,(\sigma - \mu_{t,Q,\sigma}) = [(1-\sqrt{1-t^2})/2, (1+\sqrt{1-t^2})/2]$, and

$$w_{t,0,\sigma} - U^{\mu_{t,0,\sigma}}(0) = \int_0^t g_{S(\tau)}(0)\,d\tau = -\frac{(1+t)\log(1+t)+(1-t)\log(1-t)}{2}.$$

CG, Ritz values

Example Meixner polynomials

$E_N = \{1/N, 2/N, ..., N/N, (N+1)/N, ...\} \Longrightarrow \mathrm{supp}\,(\sigma) = \Sigma = [0, +\infty)$, and σ the Lebesgue measure on $[0, +\infty)$.

By Stirling's formula, we have for $x = k/N$ and $Q(x) = -x\log(c)/2$

$$\frac{w_N(x)^{1/N}}{\exp(-Q(x))} = c^{-x/2}[\frac{c^{Nx}\Gamma(Nx+b)}{\Gamma(Nx+1)}]^{1/(2N)} = 1 + o(1)_{N\to\infty}$$

uniformly for x in some compact.

Extremal measure? Complicated, see 2.2.4, 2.3.4, or Kuijlaars & Van Assche '98:

$$\mathrm{supp}\,(\mu_{t,Q,\sigma}) = [0, \frac{1+\sqrt{c}}{1-\sqrt{c}}\,t], \qquad \mathrm{supp}\,(\sigma - \mu_{t,Q,\sigma}) = [\frac{1-\sqrt{c}}{1+\sqrt{c}}\,t, +\infty).$$

What we've learned so far

If $\nu_N(E_N) \xrightarrow{*} \sigma$ and ... details ... then

$$\limsup_{n/N \to t} E_n(z, E_N)^{1/N} \leqslant \exp\Big(-\int_0^t g_{S(\tau)}(z)\, d\tau\Big), \qquad S(t) = \mathrm{supp}\,(\sigma - \mu_{t,0,\sigma}).$$

If $\nu_N(E_N) \xrightarrow{*} \sigma$ and $w_N^{1/N} \to \exp(-Q)$ and ... details ... then

$$\limsup_{n/N \to t} \frac{1}{K_{n,2}^N(z,z)^{1/(2N)}} \leqslant \exp\Big(-(w_{t,Q,\sigma} - U^{\mu_{t,Q,\sigma}}(z))\Big).$$

Both estimates are sharp.

Rate of convergence of Krylov subspace methods and Ritz values

- Motivation, link to discrete orthogonal polynomials
- Definition of Krylov subspace methods, polynomial language
- Logarithmic potential theory (with constraint)
- Asymptotics of discrete orthogonal polynomials
- Rate of convergence of Krylov subspace methods and Ritz values
- Further examples, Applications from PDE

CG/GMRES convergence

Let $(A_N)_N$ be a sequence of symmetric invertible matrices, A_N of size $N \times N$, satisfying the conditions

(i) Asymptotic eigenvalue distribution: There exists a compact Σ and a Borel measure σ such that $\Lambda(A_N) \subset \Sigma$ for all N, and $\nu_N(\Lambda(A_N)) \xrightarrow{*} \sigma$ for $N \to \infty$;

(ii) Regularity: σ has a continuous potential;

(iii) Not too many eigenvalues too close to zero: $U^{\nu_N(\Lambda(A_N))}(0) \to U^\sigma(0)$.

Define $S(t) := \operatorname{supp}(\sigma - \mu_{t,0,\sigma})$, with the extremal measure $\mu_{t,0,\sigma}$ as before. Then for $t \in (0, \|\sigma\|)$, we have

$$\limsup_{\substack{n,N\to\infty \\ n/N\to t}} \left(\frac{\|r_{n,N}^{CG}\|_{A_N^{-1}}}{\|r_{0,N}^{CG}\|_{A_N^{-1}}} \right)^{1/n} \leqslant \limsup_{\substack{n,N\to\infty \\ n/N\to t}} E_n(0, \Lambda(A_N))^{1/n} \leqslant \exp\left(-\frac{1}{t} \int_0^t g_{S(\tau)}(0)\, d\tau \right).$$

Similarly for $||r_{n,N}^{GMRES}||/||r_{0,N}^{GMRES}||$.

Proof part 1, Proof part 2 c.f. 3.1.1, BB & Kuijlaars SINUM '00

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(ii) Regularity: σ has a continuous potential;
(iii) Not too many eigenvalues too close to zero: $U^{\nu_N(\Lambda(A_N))}(0) \to U^\sigma(0)$.
Define $S(t) := \operatorname{supp}(\sigma - \mu_{t,0,\sigma})$, with the extremal measure $\mu_{t,0,\sigma}$ as before.
Then for $t \in (0, \|\sigma\|)$, we have

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Proof part 1, Proof part 2 c.f. 3.1.1, BB & Kuijlaars SINUM '00

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Remarks CG/GMRES convergence

- A priori we do not count multiplicities of eigenvalues, but result remains valid if we do: we get conditions (i)', (ii)', (iii)'.

- Bound can roughly be written as

$$\frac{\|r_{n,N}^{CG}\|_{A_N^{-1}}}{\|r_{0,N}^{CG}\|_{A_N^{-1}}} \lessapprox \exp\Big(-N\int_0^{n/N} g_{S(\tau)}(0)\,d\tau\Big) \leqslant \prod_{j=0}^{n-1} \exp\Big(-g_{S(j/N)}(0)\Big).$$

  Notice that the factors become smaller $\Longrightarrow$ superlinear convergence.

- If $S(t) = [a(t), b(t)]$ then we get roughly

$$\frac{\|r_{n,N}^{CG}\|_{A_N^{-1}}}{\|r_{0,N}^{CG}\|_{A_N^{-1}}} \lessapprox \prod_{j=0}^{n-1} \frac{\sqrt{b(\frac{j}{N})/a(\frac{j}{N})}-1}{\sqrt{b(\frac{j}{N})/a(\frac{j}{N})}+1}.$$

  $\Longrightarrow b(\frac{j}{N})/a(\frac{j}{N})$ marginal condition number.

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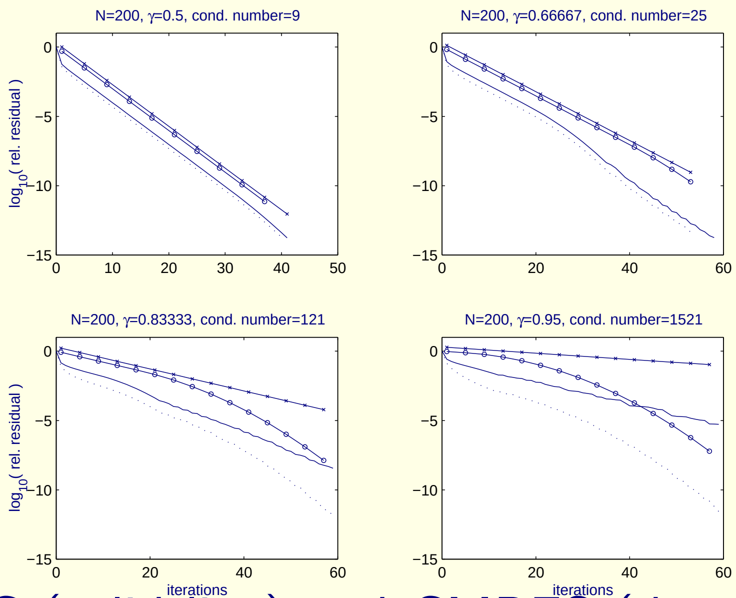
The example of Kac, Murdock and Szegő

$A_N := (\gamma^{|j-k|})_{j,k=1,2\ldots,N}$, $0 < \gamma < 1$, here (i)',(ii)',(iii)' true with $S(t) = [a, 1/a]$ for $0 < t < a := \frac{1-\gamma}{1+\gamma}$, $S(t) = [a, a/t^2]$ for $a \leqslant t < 1$.



The error curve of CG (solid line) and GMRES (dotted line) versus the classical upper bound (crosses) and our asymptotic upper bound (circles) for the system $A_{200}x = b$, with random solution x, and initial residual $r_0 = (1, ..., 1)^T$, with parameter $\gamma \in \{1/2, 2/3, 5/6, 19/20\}$.

The Poisson model problem I

Consider the two dimensional Poisson equation

$$-\frac{\partial^2 u(x,y)}{\partial x^2} - \frac{\partial^2 u(x,y)}{\partial y^2} = f(x,y)$$

for (x,y) in the unit square $0 < x, y < 1$, with Dirichlet boundary conditions on the boundary of the square.

Five-point finite difference approximation on the uniform grid

$$(j/(m_x+1), k/(m_y+1)), \qquad j = 0, 1, \ldots, m_x+1, k = 0, 1, \ldots, m_y+1,$$

leads to a system of size $N \times N$ where $N = m_x m_y$,

$$A_N = \frac{m_x+1}{m_y+1} B_{m_x} \otimes I_{m_y} + \frac{m_y+1}{m_x+1} I_{m_x} \otimes B_{m_y}, \quad B_m = \text{tridiag}(-1, 2, -1)_{m \times m}.$$

The Poisson model problem II

Since

$$A_N = \frac{m_x+1}{m_y+1} B_{m_x} \otimes I_{m_y} + \frac{m_y+1}{m_x+1} I_{m_x} \otimes B_{m_y}, \quad \lambda_k(B_m) = 2 - 2\cos\frac{\pi k}{m+1},$$

we get explicit formulas for $\lambda(A_N)$, and (i)' with

$$\sigma = \omega_{[0,4\delta]} * \omega_{[0,4/\delta]} \quad \text{for } m_x, m_y \to \infty,\ m_x/m_y \to \delta \leqslant 1.$$

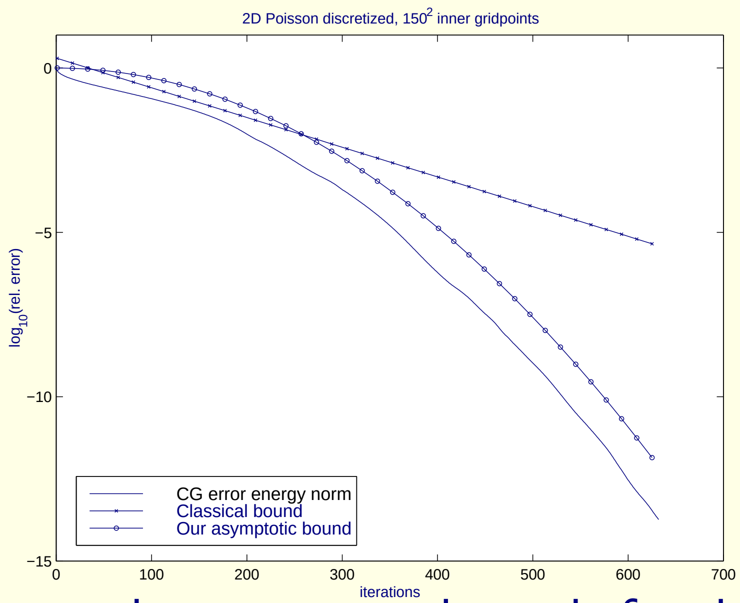
One may show with $\Delta := 2\delta + 2\delta^{-1}$

$$S(t) = [\Delta - \sqrt{\Delta^2 - 16\sin^2(\frac{\pi t}{2})}, \Delta + \sqrt{\Delta^2 - 16\sin^2(\frac{\pi t}{2})}],$$

c.f. 3.1.11 and BB & Kuijlaars SINUM '00 for $\delta = 1$.

Notice that $S(0) = [0, 2\Delta]$, $S(1) = [\delta, 1/\delta]$.

The Poisson model problem III



The CG error curve versus the two upper bounds for the system $A_N x = b$ resulting from discretizing the 2D Poisson equation on a uniform grid with $m_x = m_y = 150$. We have chosen a random solution x, and initial residual $r_0 = (1, ..., 1)^T$. For the new bound we have added a factor $1/2$ in front of σ since $\lambda_{j,k} = \lambda_{k,j}$, and we suspect that most of the eigenvalues are of multiplicity 2.

CG/GMRES convergence for special right-hand sides

Let $(A_N)_N$ be a sequence of symmetric invertible matrices, A_N of size $N \times N$, satisfying the conditions
(i), (ii), (iii) from before;
(iv) particular starting residuals: there exists a nonnegative $Q \in \mathcal{C}(\Sigma)$ such that

$$\limsup_{N\to\infty} \max_j \left[e^{Q(\lambda_{j,N})} \frac{|\beta_{j,N}|}{||r_{0,N}||} \right]^{1/N} \leqslant 1.$$

Define the extremal measure $\mu_{t,Q,\sigma}$ as before. Then for $t \in (0, \|\sigma\|)$, we have

$$\limsup_{\substack{n,N\to\infty \\ n/N\to t}} \left(\frac{\|r_{n,N}^{CG}\|_{A_N^{-1}}}{\|r_{0,N}^{CG}\|_{A_N^{-1}}} \right)^{1/N} \leqslant \exp\Big(-w_{t,Q,\sigma} + U^{\mu_{t,Q,\sigma}}(0) \Big).$$

Similarly for $||r_{n,N}^{GMRES}||/||r_{0,N}^{GMRES}||$.
Proof part 1, Proof part 2 c.f. 3.1.12, BB & Kuijlaars ETNA '02

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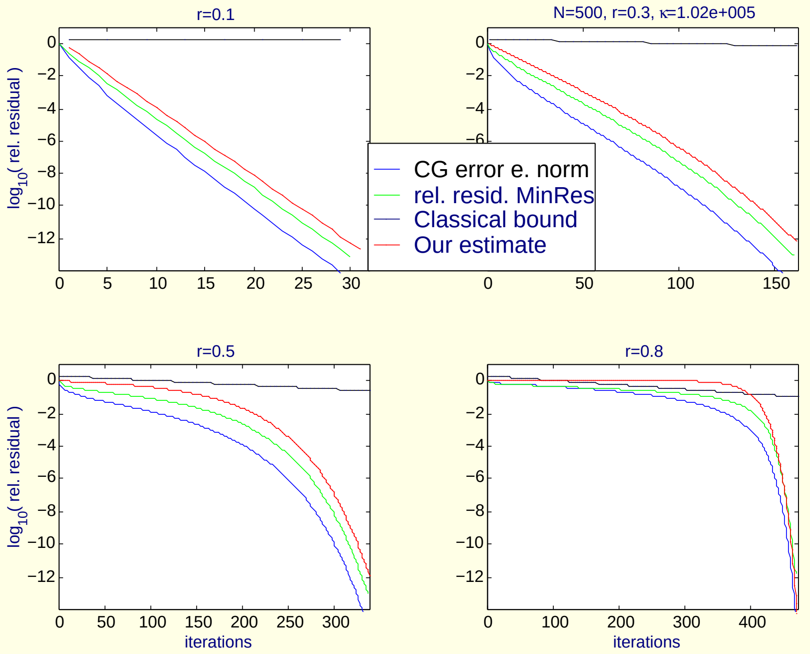
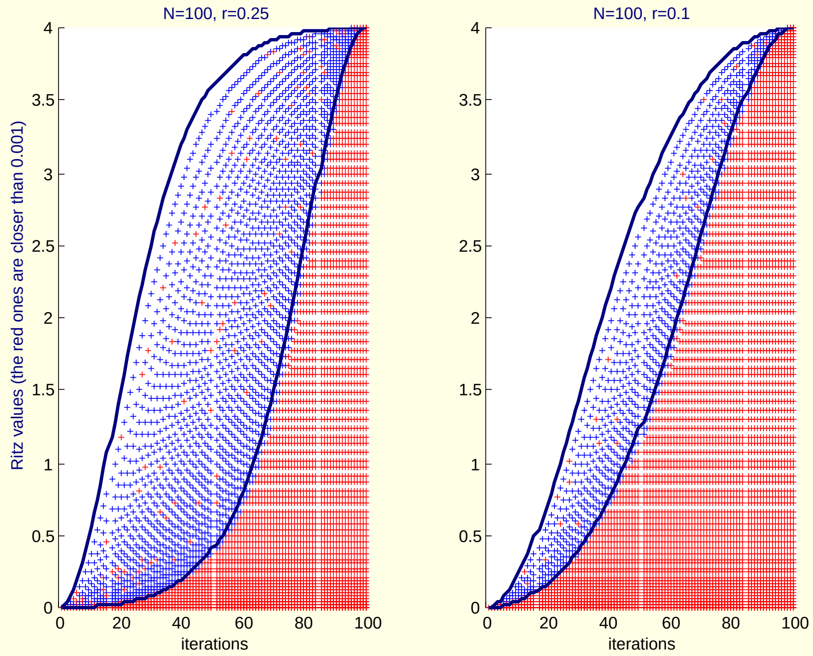
Proof part 1, Proof part 2 c.f. 3.1.12, BB & Kuijlaars ETNA '02

Example for special right-hand sides

Finite difference approximation of $-u''(x) = f(x)$ on $[0,1]$, $u(0) = u(1) = 0$.
If $f(x) = \sum_{j=1}^{\infty} f_j \sin(\pi j x)$ with $r := \limsup_{j\to\infty} |f_j|^{1/j} \in (0,1)$, then
$\sigma = \omega_{[0,4]}$, $Q(\lambda) = \frac{\log(1/r)}{\pi} \arccos(\frac{2-\lambda}{2})$, and
$w_{t,Q,\sigma} - U^{\mu_{t,Q,\sigma}}(0) = \int_0^t g_{[a(\tau),b(\tau)]}(0)\, d\tau$, with $a, b \nearrow$ (explicitly known).





Convergence of Ritz values

Let $(A_N)_N$ be a sequence of symmetric invertible matrices, A_N of size $N \times N$, satisfying the conditions (i), (ii) from before;

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$$\lim_{N\to\infty} \frac{1}{N} \sum_{j\neq k_N} \log|\lambda_{k_N,N} - \lambda_{j,N}| = \int \log|\lambda - \lambda'|\, d\sigma(\lambda'), \tag{8}$$

$$\liminf_{N\to\infty} \Big[\frac{|\beta_{k_N,N}|}{||r_{0,N}||} \Big]^{1/N} =: \rho \in (0,1]. \tag{9}$$

Define the extremal measure $\mu_{t,0,\sigma}$ as before. Then for $t \in (0, \|\sigma\|)$, we have

$$\limsup_{\substack{n,N\to\infty \\ n/N\to t}} \min_j |\lambda_{k_N,N} - x_{j,n,N}|^{1/N} \leqslant \frac{1}{\rho} \exp\Big(U^{\mu_{t,0,\sigma}}(\lambda) - w_{t,0,\sigma} \Big).$$

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$$\liminf_{N\to\infty} \Big[\frac{|\beta_{k_N,N}|}{||r_{0,N}||} \Big]^{1/N} =: \rho \in (0,1]. \tag{9}$$

Define the extremal measure $\mu_{t,0,\sigma}$ as before. Then for $t \in (0, \|\sigma\|)$, we have

$$\limsup_{\substack{n,N\to\infty \\ n/N\to t}} \min_j |\lambda_{k_N,N} - x_{j,n,N}|^{1/N} \leqslant \frac{1}{\rho} \exp\Big(U^{\mu_{t,0,\sigma}}(\lambda) - w_{t,0,\sigma} \Big).$$

Proof part 1, Proof part 2 c.f. 3.1.12, BB '02-'04

Remarks to convergence of Ritz values

- Some eigenvalues are well approximated, but some Ritz values can be far from $\Lambda(A_N)$.

- Rule of thumb (c.f. Trefethen & Bau '97): Ritz values tend to converge to eigenvalues in regions of "too little charge" σ for an equilibrium distribution $\omega_{\mathrm{supp}(\sigma)}$.
  More precisely (in case $\rho = 1$): outside the region $\cap_{\tau<t}\mathrm{supp}\,(\sigma - \mu_{t,0,\sigma})$.

- Former result with square root of right-hand bound under stronger assumptions: Kuijlaars '00a.

- If $\Sigma = [A, B]$ and if condition (vi)' with $\rho = 1$ is true uniformly for $\lambda \in [A, B')$, then for such λ we may take the square of the right-hand bound: Go back to Proof part 1

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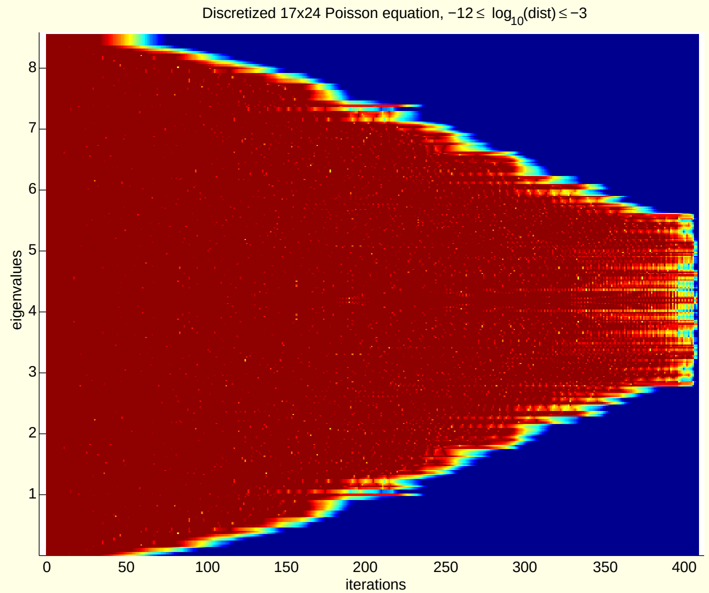
The Poisson model problem IV



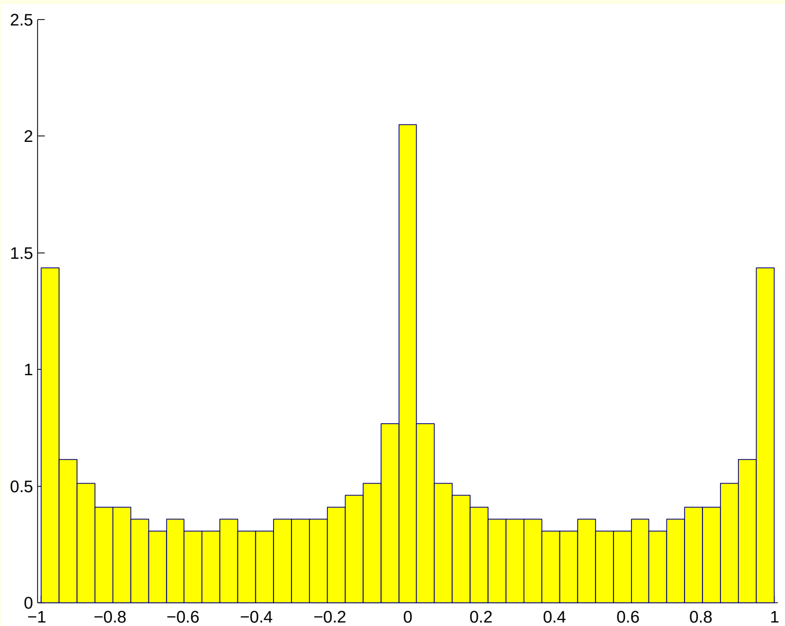
Convergence of Ritz values for the 2D Poisson problem with $m_x = 17$ and $m_y = 24$. Notice that, even for large $n \approx N$, hardly any eigenvalue in $S(1) = [4\delta, 4\delta^{-1}] = [2.83, 5.65]$ is found by Ritz values, see old results.

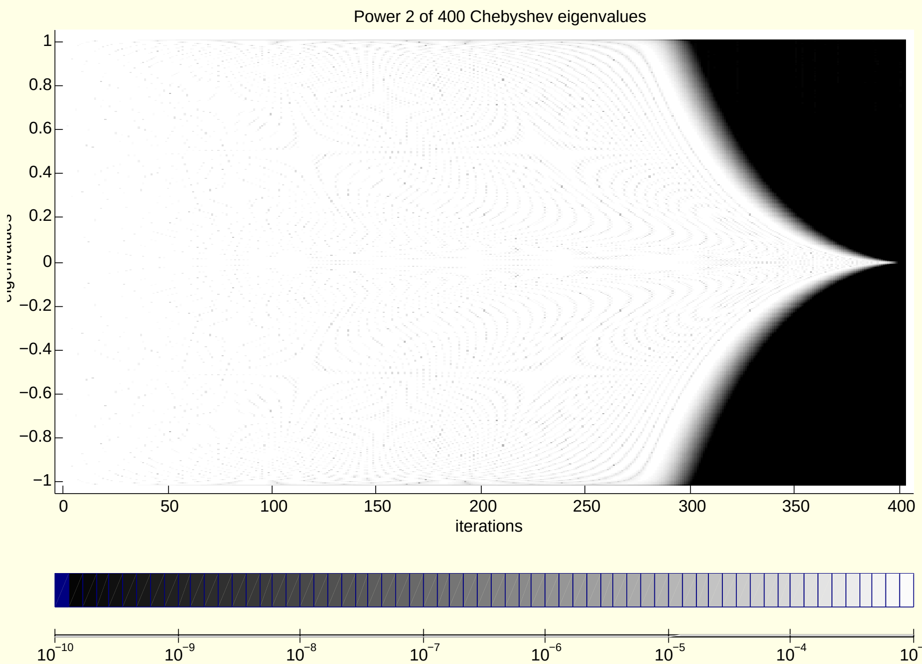
“Squares” of Chebyshev eigenvalues

Consider

$$\lambda_{j,N} = \epsilon_{j,N} \cos^2(\pi \frac{2j-1}{2N}), \quad \epsilon_{j,N} = -1 \text{ for } 2j < N \text{ and } \epsilon_{j,N} = 1 \text{ else.}$$

For $0 < t \leqslant 1/\sqrt{2}$ we obtain $S(t) = [-1, 1]$, and there is no geometric convergence of Ritz values. For $t \in (1/\sqrt{2}, 1)$, the sets are strictly decreasing and of the form $S(t) = [-b(t), b(t)]$, see the picture for $N = 400$.



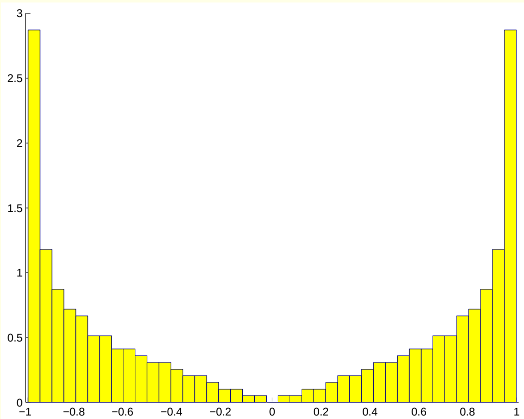


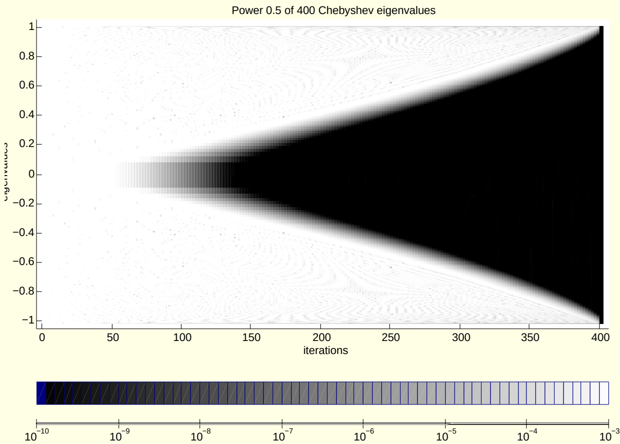
“Square roots” of Chebyshev eigenvalues

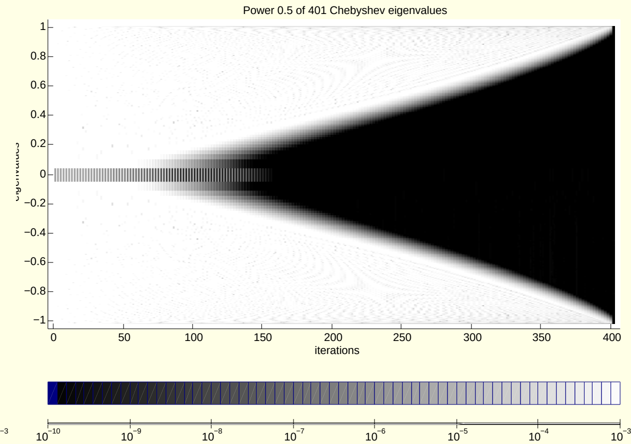
Consider

$$\lambda_{j,N} = \epsilon_{j,N}\sqrt{|\cos(\pi\frac{2j-1}{2N})|}, \quad \epsilon_{j,N} = -1 \text{ for } 2j < N \text{ and } \epsilon_{j,N} = 1 \text{ else.}$$

Here $S(t) = [-1, -r(t)] \cup [r(t), 1]$, with $r(t) = \frac{1-\cos(\pi t/2)}{1+\cos(\pi t/2)}$, see the pictures for $N = 400$ and $N = 401$.







What we should have learned

For sequences of matrices with asymptotic eigenvalue distribution σ:

- convergence of Ritz values where spectrum is not "too" dense
- rate can be quantified in terms of $\mu_{t,0,\sigma}$, solution of constrained minimal energy problem
- once an eigenvalue is matched (geometrically) by Ritz value, it can be neglected for CG or GMRES convergence
- effective condition number (= superlinear convergence) can be quantified (in weak sense) in terms of $\mu_{t,0,\sigma}$ or even $\mu_{t,Q,\sigma}$
- theory can be applied to Toeplitz matrices and systems coming from discretization of elliptic PDE

Further examples, Applications from PDE

- Motivation, link to discrete orthogonal polynomials
- Definition of Krylov subspace methods, polynomial language
- Logarithmic potential theory (with constraint)
- Asymptotics of discrete orthogonal polynomials
- Rate of convergence of Krylov subspace methods and Ritz values
- Further examples, Applications from PDE

Toeplitz matrices

$$T_N(\phi) = \begin{bmatrix} \phi_0 & \phi_1 & \cdots & \phi_{N-1} \\ \phi_{-1} & \phi_0 & \cdots & \phi_{N-2} \\ \vdots & \vdots & & \vdots \\ \phi_{1-N} & \phi_{2_N} & \cdots & \phi_0 \end{bmatrix}, \qquad \phi(\theta) = \sum_{j=-\infty}^{\infty} \phi_j e^{ij\theta}$$

$T_N(\phi) = T_N(\phi)^*$ iff $\phi_j = \overline{\phi_{-j}}$. $T_N(\phi) \geqslant 0$ iff $\phi \geqslant 0$ a.e. on $[0, 2\pi]$.

Thm: Let ϕ be real-valued and of Wiener class ($\sum |\phi_j| < \infty$), then (H1)' holds,

$$\text{with} \qquad \int f d\sigma = \frac{1}{2\pi} \int_0^{2\pi} f(\phi(e^{i\theta}))\, d\theta.$$

Moreover, if $\phi \geqslant 0$, then (H2)' implies (H3)'.

Remark: A similar result is true for level 2 Toeplitz matrices (each entry is again Toeplitz) with symbol having absolutely convergent Fourier series.

Idea of proof

Step 1 (make T_N banded): Let $\phi^{(k)}$ be partial sum of ϕ, then

$$\lim_k \sup_N ||T_N(\phi) - T_N(\phi^{(k)})|| \leqslant \lim_k \sum_{|j|>k} |\phi_j| = 0.$$

Step 2 (transform to circulants): let

$$C_{k,N} = \begin{bmatrix} \phi_0 & \phi_1 & \cdots & \phi_k & 0 & 0 & \cdots & 0 & \phi_{-k} & \phi_{1-k} & \cdots & \phi_{-1} \\ \phi_{-1} & \phi_0 & \cdots & \phi_{k-1} & \phi_k & 0 & \cdots & 0 & 0 & \phi_{-k} & \cdots & \phi_{-2} \\ \vdots & \ddots & \ddots & & \ddots & \ddots & \ddots & & \ddots & \ddots & & \end{bmatrix}.$$

For fixed k, (asymptotic) spectrum of $(C_{k,N})_N$ is known (FFT), given by $\sigma^{(k)}$, and rank$(C_{N,k} - T_N(\phi^{(k)})) \leqslant 2k$.

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Idea of proof (continued)

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$\sigma^{(k)} \xrightarrow{*} \sigma$ for $k \to \infty$.

Step 4: (H2)' implies that

$$\infty > U^\sigma(0) = -\int \log(\phi^{i\theta})\, d\theta \qquad \Longrightarrow$$

$$\frac{\det(T_N(\phi))}{\det(T_{N-1}(\phi))} \to -U^\sigma(0) \qquad \Longrightarrow$$

$$|\det(T_N(\phi))|^{1/N} \to -U^\sigma(0) \qquad \Longrightarrow \text{(H3)'}$$

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Diffusion problem I

Let $\Omega \subset [0,1]^2$ be some open polyhedron, and $b : \Omega \to [0, +\infty)$ piecewise continuous. Discretize

$$\text{div}(b\nabla u) = f \quad \text{on } \Omega$$

plus Dirichlet (Neumann) boundary conditions via central finite differences with stepsizes

$$\Delta x = \frac{1}{m_x + 1}, \quad \Delta y = \frac{1}{m_y + 1}, \quad m_x, m_y \to \infty, \quad \frac{m_x}{m_y} \to \delta < 1.$$

Leads to system

$$A_N x = b_N.$$

Remark: (Discretization of) BC not so important, small rank pertubation of order $\mathcal{O}(\sqrt{N})$.

Diffusion problem II

Thm: We have

$$\lim_{N\to\infty} \int f \, d\nu_N(A_N) =$$

$$\frac{1}{m(\Omega)} \int_\Omega dx \frac{1}{(2\pi)^2} \iint_{[0,2\pi]^2} ds \, f(b(x) \cdot [2\delta(1-\cos(s_1)) + 2\delta^{-1}(1-\cos(s_2))])$$

with $m(\cdot)$ denoting the two-dimensional Lebesgue measure.

Idea of proof:

- cut Ω in squares, replace b on each square by constant;
- use 3.1.11 on each square, apply the perturbation result.

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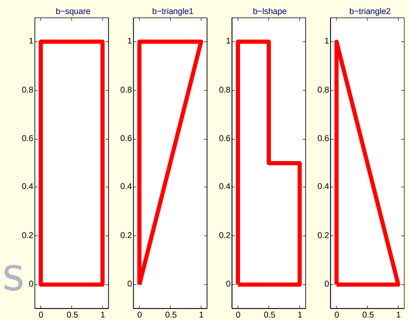
Diffusion problem III

- more general result on FD discretization given by Serra Capizzano;
- Relation to Weyl formula

$$\sigma'(y) = \frac{1}{4\pi\, m(\Omega)} \int_\Omega \frac{dx}{b(x)} + y \frac{\delta + \delta^{-1}}{32\pi\, m(\Omega)} \int_\Omega \frac{dx}{b(x)^2} + \mathcal{O}(y^2)_{y \to 0}.$$

- Numerical experiments for four domains



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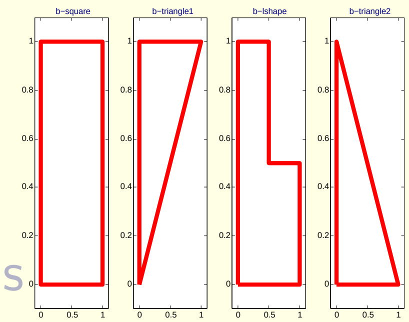

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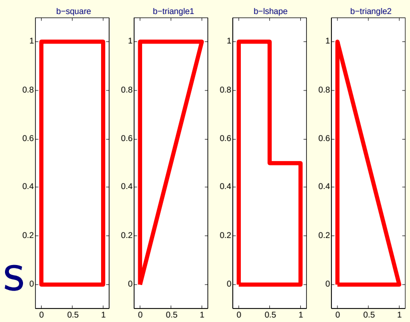
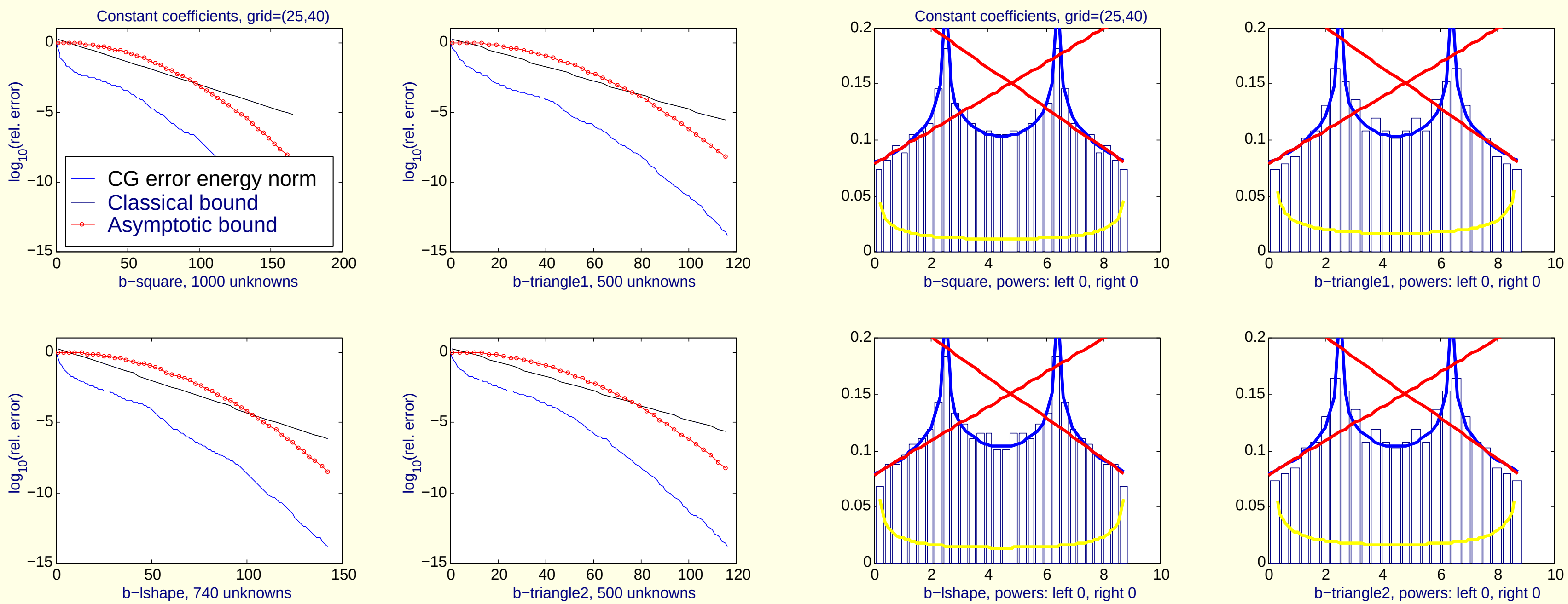


Diffusion problem IV



Diffusion problem V