

Monotone Convergence of the Spectral Lanczos Decomposition Method

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Outline

- ▶ Lanczos etc.
- ▶ $\exp(A)b$
- ▶ Other Functions: $A^{-1}b$ and Stieltjes Transforms
- ▶ Bonus: Error Bounds for Rational Functions
- ▶ Conclusions



The Setting

Always:

- ▶ $A \in \mathbb{C}^{n \times n}$ *hermitian*
- ▶ $f : D \subseteq \mathbb{C} \rightarrow \mathbb{C}$, $\text{spec}(A) \subseteq D$



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- ▶ A *hermitian and positive definite*
- ▶ f *special*, for example *exp*, *sign*, *inverse square root*, ...



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Problem:

- ▶ given $b \in \mathbb{C}^n$
- ▶ compute approximations u^m to $u = f(A)b$



The Lanczos Process (I)

Krylov subspace: $K_m(A, b) = \text{span}\{b, Ab, \dots, A^{m-1}b\}$

Lanczos vectors: $\{v^1, \dots, v^m\}$ is an orthon. basis of $K_m(A, b)$

Lanczos process:

for $m = 1, \dots, m_{max}$

$$\beta_m = \|\tilde{v}^m\|$$

$$v^m = \tilde{v}^m / \beta_m$$

$$\tilde{w}^{m+1} = Av^m - \beta_m v^{m-1}$$

$$\alpha_m = \langle \tilde{w}^{m+1}, v^m \rangle$$

$$\tilde{v}^{m+1} = \tilde{w}^{m+1} - \alpha_m v^m$$



The Lanczos Process (II)

Summary:

$$AV_m = V_m T_m + \beta_{m+1} v_{m+1} e_m^T,$$

where

$$V_m = [v^1 | \dots | v^m] \in \mathbb{C}^{n \times m}$$

e_m is the m -th Cartesian unit vector in \mathbb{C}^m

T_m is symmetric tridiagonal

$$T_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & & \beta_m & \alpha_m \end{bmatrix} = V_m^* A V_m$$



Spectral Lanczos Decomposition Method

Approximate:

$$\begin{aligned} u^m &= V^m \cdot f((V^m)^* A V^m) \cdot (V^m)^* b \\ &= V^m \cdot f(T_m) \cdot (\beta_1 e^1), \quad \beta_1 = \|b\| \end{aligned}$$



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Note:

- ▶ $u^m \in K_m(A, b)$
- ▶ If $f(z) = z^{-1}$, SLDM = CG with $x^0 = 0$
- ▶ Method occurs since the mid 80s
- ▶ Relation to polynomial interpolation etc.



A First Idea for Monotone Convergence

Observation: $f(A)b = u^{m_{\max}} = V^{m_{\max}} \cdot f(T_{m_{\max}}) \cdot (\beta_1 e_1)$

Define:

- ▶ coefficient vector for u^m w.r.t. Lanczos basis:

$$s^m = f(T_m) \cdot (\beta_1 e_1)$$

- ▶ ℓ_2 -norm of error:

$$\|u - u^m\| = \|s^{m_{\max}} - s^m\|$$

Sufficient condition for $\|u - u^m\| \downarrow 0$: $0 \leq \begin{pmatrix} s^m \\ 0 \end{pmatrix} \leq s^{m+1}$

Side result: $\|u^m\| \uparrow \|f(A)b\|$



Assume A hermitian positive definite

Power series representation: $\exp(T_m) = \sum_{i=0}^{\infty} \frac{1}{i!} (T_m)^i$

Notation: $\hat{T}_m = \begin{bmatrix} T_m & \mathbf{0} \\ \mathbf{0}^T & * \end{bmatrix}$

Crucial observation:

$$0 \leq \hat{T}_m \leq T_{m+1} \implies 0 \leq \hat{T}_m^i \leq T_{m+1}^i \text{ for all } i$$

Consequence:

$$0 \leq \begin{pmatrix} s^m \\ 0 \end{pmatrix} = \left(\sum_{i=0}^{\infty} \frac{1}{i!} (\hat{T}_m)^i \right) \cdot \beta_1 \mathbf{e}_1 \leq \left(\sum_{i=0}^{\infty} \frac{1}{i!} (T_m)^i \right) \cdot \beta_1 \mathbf{e}_1 = s^{m+1}$$



Results for $\exp(A)b$

Theorem: Let A be hermitian positive definite,
 $u^m = V_m f(T_m) \cdot (\beta_1 e_1)$, $u = f(A)b$. Then

$$\|u^m - u\| \downarrow 0, \quad \|u^m\| \uparrow \|u\|.$$



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Corollary [Druskin, 2008]: Theorem also holds if A is just hermitian.

Proof. Choose $\alpha > 0$ s.t. $\tilde{A} = A + \alpha I$ is positive definite and use

$$\tilde{T}_m = T_m + \alpha I$$

and

$$\exp(\tilde{A}) = e^\alpha \cdot \exp(A).$$



$$f(z) = z^{-1}: \text{SLDM} = \text{CG}$$

Consider

$$f(z) = z^{-1}, \quad u = A^{-1}b, \quad A \text{ pos. def.}$$

- ▶ pole at $z = 0$
- ▶ power series approach does not work



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We know from school: $\|u^m - u\|_A \downarrow 0$ and $\|u^m - u\|_2 \downarrow 0$

Can we see this from the coefficients $s^m = T_m^{-1} \cdot (\beta_1 e_1)$?



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Answer: Yes, since

$$0 \leq s_i^m \leq s_i^{m+1} \quad \text{for } i \text{ odd}$$

$$0 \geq s_i^m \geq s_i^{m+1} \quad \text{for } i \text{ even}$$



Proof (I)

Redefine Lanczos vectors:

$$v_m^\pm = (-1)^{m-1} v_m,$$

$$V_m^\pm = [v_1^\pm | \dots | v_m^\pm] = V_m \cdot S, \quad S = \text{diag}(1, -1, \dots)$$

Then $T_m = V_m^* A V_m \implies T_m^\pm = (V_m^\pm)^* A V_m^\pm = S T_m S$

with

$$T_m^\pm = \begin{bmatrix} \alpha_1 & -\beta_2 & & & & \\ -\beta_2 & \alpha_2 & -\beta_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & -\beta_{m-1} & \alpha_{m-1} & -\beta_m \\ & & & & -\beta_m & \alpha_m \end{bmatrix}$$



Proof (II)

$$T_m^\pm = ST_mS$$

Consequence: T_m^\pm is hermitian positive definite with non-positive offdiagonal

$\implies T_m^\pm$ is a *Stieltjes matrix*, i.e. a hermitian positive definite M-matrix. In particular,

$$(T_m^\pm)^{-1} \geq 0.$$



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Useful facts: Let $B, C \in \mathbb{R}^{m \times m}$ be two M-matrices and let $E \in \mathbb{R}^{m \times m}$ be such that $E \geq 0$.

- (i) If $B \leq C$ then $0 \leq C^{-1} \leq B^{-1}$.
- (ii) If $B + E$ has all its offdiagonal entries nonpositive, then $B + E$ is an M-matrix.



Proof (III)

$$u^m = V_m \cdot T_m^{-1} \cdot (\beta_1 e_1) = V_m^\pm \cdot (T_m^\pm)^{-1} \cdot (\beta_1 e_1)$$

Study coefficient vector w.r.t. V_m^\pm , i.e.

$$s^m = (T_m^\pm)^{-1} \cdot (\beta_1 e_1)$$

Define:

$$\hat{T}_{m+1}^\pm = \begin{bmatrix} T_m^\pm & \mathbf{0} \\ \mathbf{0}^T & \alpha_{m+1} \end{bmatrix}$$



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Then $T_{m+1} \leq \hat{T}_{m+1}^\pm$ and $0 \leq (\hat{T}_{m+1}^\pm)^{-1} \leq (T_{m+1}^\pm)^{-1}$ and

$$0 \leq \begin{pmatrix} s^m \\ \end{pmatrix} = (\hat{T}_{m+1}^\pm)^{-1} \cdot \beta_1 e_1 \leq (T_{m+1}^\pm)^{-1} \cdot \beta_1 e_1 = s^{m+1}$$



Did you know ...



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$$\|u^m\| \uparrow \|A^{-1}b\|$$

if one starts CG with $u^0 = 0$?

[Steihaug, 1983]



Generalization

Assume

$$f(z) = \int_{t=0}^{\infty} \frac{1}{(t+z)^k} d\mu \quad \text{for } z > 0, \quad (1)$$

where μ is a non-negative measure s.t. $\int_1^{\infty} \frac{1}{t^k} d\mu$ is finite.



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Theorem: Let A be positive definite and f be of the form (1). Then the SLDM approximations u^m for $u = f(A)b$ satisfy

$$\|u - u^m\| \downarrow 0, \quad \|u^m\| \uparrow \|u\|.$$

Proof: The coefficient vectors s^m can be expressed as

$$s^m = \int_{t=0}^{\infty} (tl + T_m^{\pm})^{-k} d\mu \cdot (\beta_1 e_1).$$

Use same arguments as before for M-matrices $tl + T_m^{\pm}$.



Special Cases (I)

Corollary: Monotone convergence for

▶ $f(z) = z^{-k}$, $k \in \mathbb{N}$,

▶ $f(z) = \sum_{i=1}^p \frac{\alpha_i}{z + \beta_i}$ with $\alpha_i \geq 0, \beta_i > 0$ for $i = 1, \dots, p$,

▶ $f(z) = \sum_{i=1}^{\infty} \frac{\alpha_i}{z + \beta_i}$ with $\alpha_i \geq 0, \beta_i > 0$ for $i = 1, 2, \dots$ and

$$\lim_{i \rightarrow \infty} \beta_i = \infty, \lim_{i \rightarrow \infty} |\alpha_i / \beta_i| < \infty,$$

▶ $f(z) = z^{-\alpha}$ for $\alpha \in (0, 1)$,

▶ $f(z) = z^{-\alpha}(1+z)^{-\beta}$, $0 < \alpha \leq 1, \alpha + \beta \in [0, 1)$,

▶ $f(z) = (z-1)^{-1} \log z$,



Special Cases (II)

- ▶ f is the result of a Stieltjes transform, i.e.

$$f(z) = \int_{t=0}^{\infty} \frac{1}{z+t} d\mu(t),$$

where μ is a nonnegative measure such that $\int_1^{\infty} \frac{1}{t} d\mu(t) < \infty$,

- ▶ $f(z) = \sum_{i=1}^{\ell} \gamma_i f_i(z)$ with $\gamma_i \geq 0$ for all i and f_i any function from before or a constant.

Note: $f : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is the result of a Stieltjes transform
iff

f can be extended to a holomorphic function on $\mathbb{C} \setminus (-\infty, 0]$ which maps the upper half plane to the lower half plane.



Extensions

Situation:

- ▶ $f(z) = g(z) \cdot h(z)$
- ▶ $h(A)b$ directly computable, e.g. h a polynomial

Theorem: Assume $f(z) = g(z) \cdot h(z)$ with g from previous theorems. Compute $u = f(A)b$ as

$$u = g(A) \cdot (h(A)b), \quad u^m = V^m g(T_m) \cdot (h(A)b).$$

Then $\|u - u^m\| \downarrow 0$, $\|u^m\| \uparrow \|u\|$.



Sign Function

Assume A hermitian, *indefinite*

$$f(z) = \text{sign}(z) = (z^2)^{-1/2} \cdot z.$$

Compute $u = \text{sign}(A)b$ as

$$u = B^{-1/2} \cdot c \quad \text{with } B = A^2, c = Ab,$$

$$u^m = (T_m)^{-1/2} \cdot c \quad \text{where } T_m \text{ is w.r.t. } B = A^2$$

Then again:

$$0 \leq \begin{pmatrix} s^m \\ 0 \end{pmatrix} = (\hat{T}_{m+1}^\pm)^{-1/2} \cdot \beta_1 e_1 \leq (T_{m+1}^\pm)^{-1/2} \cdot \beta_1 e_1 = s^{m+1}$$



Error Bounds for Sign Function

Note: For A hermitian, $\text{sign}(A)$ is unitary. Thus

$$\|\text{sign}(A)b\| = \|b\|.$$

So we know $\|u^m\| \uparrow \|b\|$.

Theorem: Assume A is hermitian, compute u^m as on previous slide. Then

$$\|b\| - \|u^m\| \leq \|u - u^m\| \leq (\|b\|^2 - \|u^m\|^2)^{1/2}.$$

Proof: Minimize and maximize

$$\|t - s^m\|$$

under the constraints

$$t \geq s^m, \|t\| = \|b\|.$$



Error Bounds for Rational Functions

Assume:

$$f(z) = \sum_{i=1}^p \frac{\omega_i}{z - \sigma_i}$$

Facts:

- ▶ $u^m = V_m^* \cdot (\sum_{i=1}^p \omega_i (T_m - \sigma_i I)^{-1}) \cdot \beta_1 e_1$
- ▶ $V_m^* \cdot (T_m - \sigma_i I)^{-1} \cdot \beta_1 e_1$ is CG iterate x_i^m for system $(A - \sigma_i I)x = b$
- ▶ Residuals $r_i^m = b - (A - \sigma_i I)x_i^m$ are collinear,

$$r_i^m = (-1)^{m-1} \rho_i^m v_m, \quad \rho_i^m = \|r_i^m\|$$

Consequence: $u - u^m = \left(\sum_{i=1}^s \omega_i \rho_i^m (A - \sigma_i I)^{-1} \right) v^m .$



$$u - u^m = \left(\sum_{i=1}^s \omega_i \rho_i^m (A - \sigma_i I)^{-1} \right) v^m$$

Thus:

$$\|u - u^m\| \leq \lambda_{\max}^{(m)}, \quad \|u - u^m\| \geq \lambda_{\min}^{(m)},$$

$\lambda_{\min}^{(m)}$ smallest, $\lambda_{\max}^{(m)}$ largest (in modulus) eigenvalue of

$$H^{(m)} = \sum_{i=1}^s \omega_i \rho_i^m (A - \sigma_i I)^{-1}.$$

If $\text{spec}(A) \subseteq [a, b]$, we have

$$\lambda_{\min}^{(m)} \geq \min_{t \in [a, b]} \left| \sum_{i=1}^s \frac{\omega_i \rho_i^m}{t - \sigma_i} \right|, \quad \lambda_{\max}^{(m)} \leq \max_{t \in [a, b]} \left| \sum_{i=1}^s \frac{\omega_i \rho_i^m}{t - \sigma_i} \right|$$



Error bounds

Error bounds:

$$\|u - u^m\| \geq \min_{t \in [a, b]} \left| \sum_{i=1}^s \frac{\omega_i \rho_i^m}{t - \sigma_i} \right|$$
$$\|u - u^m\| \leq \max_{t \in [a, b]} \left| \sum_{i=1}^s \frac{\omega_i \rho_i^m}{t - \sigma_i} \right|.$$

Bounds for the rhs via (interval) global optimization for

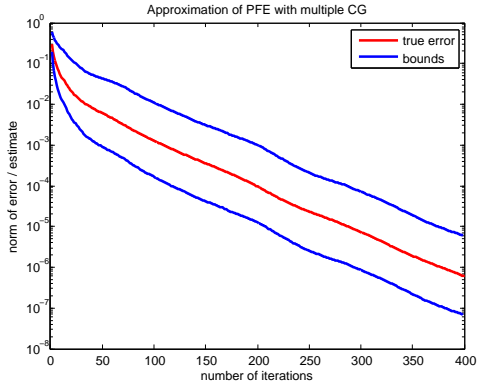
$$h(t) = \left| \sum_{i=1}^s \frac{\omega_i \rho_i^m}{t - \sigma_i} \right|$$

Work does not depend on A nor its dimension



Computational results (I)

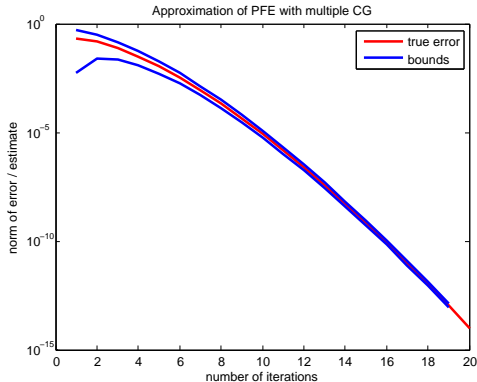
Example 1: $\text{sign}(Q)b$ as $\sum_{i=1}^s \omega_i \cdot Q \cdot (Q^2 - \sigma_i I)^{-1} b$.
QCD matrix of size $12 \cdot 8^4$





Computational results (II)

Example 2: $\exp(-Q)b$ as $\sum_{i=1}^s \omega_i l \cdot (Q - \sigma_i)^{-1} b$.
2d Laplacian of 40×40 grid





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- ▶ Monotone convergence for Stieltjes transforms
- ▶ includes / extends to rational functions, sign function
- ▶ error bounds for sign
- ▶ Open question: shift and invert preconditioning