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*
- $f : D \subseteq \mathbb{C} \to \mathbb{C}$, $\text{spec}(A) \subseteq D$

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

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

Lanczos process:

for $m = 1, \ldots, m_{max}$
$\beta_m = \|\tilde{v}^m\|$
$v^m = \tilde{v}^m / \beta_m$
$\tilde{w}^{m+1} = Av^m - \beta_m v^{m-1}$
$\alpha_m = \langle \tilde{w}^{m+1}, v^m \rangle$
$\tilde{v}^{m+1} = \tilde{w}^{m+1} - \alpha_m v^m$

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), \;\; \beta_1 = \|b\|
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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 $\|u - u^m\| \downarrow 0$: $0 \le \begin{pmatrix} s^m \\ 0 \end{pmatrix} \le s^{m+1}$

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

Crucial observation:

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

Consequence:

$$0 \le \begin{pmatrix} s^m \\ 0 \end{pmatrix} = \left(\sum_{i=0}^{\infty} \frac{1}{i!} (\hat{T}_m)^i \right) \cdot \beta_1 e_1 \le \left(\sum_{i=0}^{\infty} \frac{1}{i!} (T_m)^i \right) \cdot \beta_1 e_1 = s^{m+1}$$

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

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

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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

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

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

$$\begin{aligned} 0 \le s_i^m \le s_i^{m+1} \qquad & \text{for } i \text{ odd} \\ 0 \ge s_m^i \ge s_i^{m+1} \qquad & \text{for } i \text{ even} \end{aligned}$$

Proof (I)

Redefine Lanczos vectors:

$$v_m^{\pm} = (-1)^{m-1} v_m,$$
$$V_m^{\pm} = \left[v_1^{\pm} | \dots | v_m^{\pm} \right] \; = \; V_m \cdot S, \; S = \operatorname{diag}(1, -1, \dots)$$

Then $T_m = V_m^* A V_m \Longrightarrow T_m^{\pm} = (V_m^{\pm})^* A V_m^{\pm} = S T_m S$

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)

$$T_m^{\pm} = S T_m S$$

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

$\Longrightarrow$ $T_m^{\pm}$ 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:

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

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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

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

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

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

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

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 $i = 1, \ldots, p$,
- $f(z) = \sum_{i=1}^{\infty} \frac{\alpha_i}{z+\beta_i}$ with $\alpha_i \geq 0, \beta_i > 0$ for $i = 1, 2, \ldots$ and $\lim_{i\to\infty} \beta_i = \infty, \lim_{i\to\infty} |\alpha_i/\beta_i| < \infty$,
- $f(z) = z^{-\alpha}$ 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: $f : \mathbb{R}^+ \to \mathbb{R}^+$ 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*

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

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:

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

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

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

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:

- $u^m = V_m^* \cdot \left(\sum_{i=1}^{p} \omega_i (T_m - \sigma_i I)^{-1}\right) \cdot \beta_1 e_1$
- $V_m^* \cdot (T_m - \sigma_i I)^{-1} \cdot \beta_1 e_1$ 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: $u - u^m = \left(\sum_{i=1}^{s} \omega_i \rho_i^m (A - \sigma_i I)^{-1} \right) v^m$.

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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 $\mathrm{spec}(A) \subseteq [a, b]$, 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:

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

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

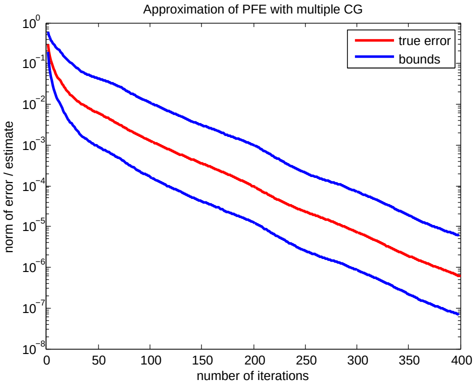
Bounds for the rhs via (interval) global optimization for

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

Work does not depend on A nor its dimension

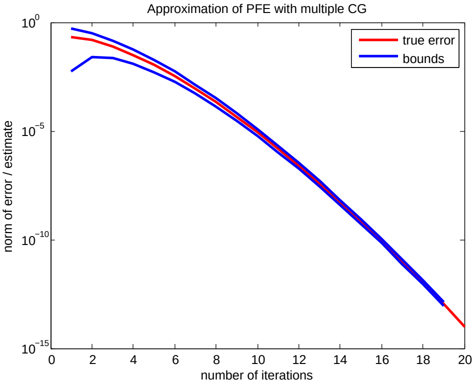
Computational results (I)

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



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- Open question: shift and invert preconditioning