Field of values error estimates for evaluating functions of matrices via the Arnoldi method

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Outline

- the problem: approaching $g(A)b$ via Arnoldi's method
- here: error estimates in terms of field of values $W(A) = \{y^*Ay : \|y\| = 1\}$
- link with best polynomial approximation of g on $W(A)$?
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Outline

- the problem: approaching $g(A)b$ via Arnoldi's method
- here: error estimates in terms of field of values
  $W(A) = \{y^*Ay : \|y\| = 1\}$
- link with best polynomial approximation of g on $W(A)$?

- Explicit bounds for $\exp(A)b$
- Explicit bounds for $A^\kappa b$, $-1 < \kappa < 0$, and other Markov functions
- Explicit bounds for general powers and $\log(A)b$

The problem

How to approximately compute $g(A)b$, where

$$\|b\| = 1, \quad A \in \mathbb{C}^d \text{ large, sparse, non-symmetric...?}$$

Arnoldi decomposition

$$AV_m = V_m H_m + f_m e_m^*, \quad H_m \in \mathbb{C}^m \text{ upper Hessenberg,}$$

and $V_m \in \mathbb{C}^{d\times n}$, $V_m^* V_m = I_m$, $V_m e_1 = b$, $V_m^* f_m = 0$.

We have for each polynomial p of degree $< m$:
$p(A)b = p(A)V_m e_1 = V_m p(H_m) e_1$.

Approximation via Arnoldi:

- compute Arnoldi decomposition V_m, H_m for "small" m
- compute exactly $g(H_m)$
- approach $g(A)b$ by $V_m g(H_m) e_1$.

Error estimate with Crouzeix

For each polynomial p of degree $< m$

$$\begin{aligned} \|g(A)b - V_m g(H_m)e_1\| &= \|(g-p)(A)b - V_m(g-p)(H_m)e_1\| \\ &\leq \|(g-p)(A)\| + \|(g-p)(H_m)\|. \end{aligned}$$

THEOREM 1: Let $\mathbb{E} \subset \mathbb{C}$ be some convex and compact set containing the field of values

$$W(A) = \{y^* A y : y \in \mathbb{C}^d, \|y\| = 1\},$$

and let g be analytic on $\mathbb{E}$, then

$$\|g(A)b - V_m g(H_m)e_1\| \leq 24\, \eta_m(g, \mathbb{E}), \qquad \eta_m(g, \mathbb{E}) := \min_{\deg p < m} \|g - p\|_{L_\infty(\mathbb{E})}.$$

Proof: Michel Crouzeix in 2006 showed that $\|f(B)\| \leq 12\, \|f\|_{L_\infty(W(B))}$.
Also, $H_m = V_m^* A V_m \Longrightarrow W(H_m) \subset \mathbb{E}$. □

Riemann maps and Faber maps

Let $\mathbb{E}$ convex and compact as before, $\mathbb{D}$ the closed unit disc, then there exists unique conformal maps $\phi : \mathbb{E}^c \mapsto \mathbb{D}^c$ with $\phi(\infty) = \infty$, $\phi'(\infty) > 0$, $\psi := \phi^{-1}$.

Level sets for $R > 1$ defined by complement: $\mathbb{E}_R^c = \{z \in \mathbb{E}^c : |\phi(z)| > R\}$.

Bernstein Theorem: If g analytic in $\mathbb{E}_R$ then

$$\eta_m(g, \mathbb{E}) = \min_{\deg p < m} \|g - p\|_{L_\infty(\mathbb{E})} \le 2 \frac{R^{-m}}{1 - R^{-1}} \|g\|_{L_\infty(\mathbb{E}_R)}.$$

Faber map $\mathcal{F} : \mathcal{A}(\mathbb{D}) \mapsto \mathcal{A}(\mathbb{E})$ defined by

$$\mathcal{F}(G)(z) = \frac{1}{2\pi i} \int_{|w|=1} \frac{\psi'(w)}{\psi(w) - z} G(w)\, dw.$$

$$g = \mathcal{F}(G) \quad \Longrightarrow \quad \frac{1}{\|\mathcal{F}^{-1}\|} \eta_m(G, \mathbb{D}) \le \eta_m(g, \mathbb{E}) \le 2\, \eta_m(G, \mathbb{D}).$$

Faber polynomials and Faber series

Faber polynomial: $F_n(z) = \mathcal{F}(w^n)(z)$ polynomial of degree n,
F_n polynomial part of ϕ^n,
Pommerenke and Kővari '67 ($\mathbb{E}$ convex): $\|F_n - \phi^n\|_{L_\infty(\mathbb{E})} \leq 1$.

Examples: $\mathbb{E} = a + \mathbb{D}_R$: $F_n(z) = (\frac{z-a}{R})^n$.
$\mathbb{E} = [-1, 1]$: $F_n(z) = 2T_n(z)$ Chebyshev polynomials of first type.

Faber series: For $g \in \mathcal{A}(\mathbb{E})$, $j \geq 0$

$$g_j = \frac{1}{2\pi i} \int_{|w|=1} \frac{g(\psi(w))}{w^{j+1}} \, dw \quad \Longrightarrow \quad g = \mathcal{F}(G), \quad G(w) = \sum_{j=0}^{\infty} g_j w^j,$$

where the last sum, and $g(z) = \sum_{j=0}^{\infty} g_j F_j(z)$, are absolutely convergent in $\mathbb{D}$, and $\mathbb{E}$, respectively.

THEOREM 2: Let $\mathbb{E} \subset \mathbb{C}$ be some convex and compact set containing the field of values $W(A)$ and let $g = \mathcal{F}(G)$ be analytic on $\mathbb{E}$, then

$$\|g(A)b - V_m g(H_m)e_1\| \leq 4\, \eta_m(G, \mathbb{D}).$$

Idea of proof of Theorem 2

Inspired from Crouzeix, Delyon, Badea, BB 02-07, in particular the CRAS '05 of BB: $\|F_n(A)\| \leq 2$. It is sufficient to show

$$\|h(A)\| \leq 2\|H\|_{L_\infty(\mathbb{D})}, \quad h = \mathcal{F}(H) + H(0).$$

Here $W(A) \subset \text{Int}(\mathbb{E})$ for simplicity. We have

$$\mathcal{F}(w^m)(A) = \frac{1}{2\pi i}\int_{|w|=1} w^m \psi'(w)(\psi(w)-A)^{-1}dw = \begin{cases} F_m(A) & \text{if } m = 0, 1, 2, \ldots, \\ 0 & \text{if } m = -1, -2, \ldots. \end{cases}$$

Hence

$$h(A) = \frac{1}{2\pi}\int_{|w|=1} H(w)\left(\underbrace{\left(w\psi'(w)(\psi(w)-A)^{-1}\right) + \left(w\psi'(w)(\psi(w)-A)^{-1}\right)^*}_{\text{positive definite}}\right)\frac{dw}{iw}.$$

How to exploit Theorem 2?

$$\|g(A)b - V_m g(H_m)e_1\| \leq 4\,\eta_m(G,\mathbb{D}), \quad g(z) = \sum_{j=0}^{\infty} g_j F_j(z), \quad G(w) = \sum_{j=0}^{\infty} g_j w^j.$$

LEMMA 3:

$$\left.\begin{array}{l} |g_m| \\ |g_m + g_{m+(m+1)} + g_{m+2(m+1)} + ...| \\ |g_m - g_{m+(m+1)} + g_{m+2(m+1)} \mp ...| \end{array}\right\} \leq \eta_m(G,\mathbb{D}) \leq \sum_{j=0}^{\infty} |g_{m+j}|.$$

Knitznerman '91 gave a similar upper bound with additional powers of $m+j$
Hochbruck & Lubich '97 gave a more complicated bound, weaker up to factor 0.75.

Idea of proof: Upper bound partial sum. First lower bound

$$\deg q < m: \qquad g_m = \frac{1}{2\pi i}\int_{|w|=1} \frac{G(w)}{w^{m+1}}\,dw = \frac{1}{2\pi i}\int_{|w|=1} \frac{G(w)-q(w)}{w^{m+1}}\,dw.$$

For second lower bound compute $\eta_m(G, \{\exp(\frac{2\pi i j}{m+1}) : j = 0,1,...,m\})$ = modulus of leading coefficient of interpolating polynomial at these roots of unity. □

Application 1: the exponential function

Consider $\mathbb{E}$ symmetric with respect to real axis (e.g., $A \in \mathbb{R}^{d\times d}$), and $g(z) = \exp(\tau z)$, $\tau > 0$. We write $\psi(w) = \text{cap}(\mathbb{E})w + c + \mathcal{O}(1/[w|)_{|w|\to\infty}$.

LEMMA 4: the case of "large" j: there exist explicit "modest" constants $K, K_1, K_2 > 0$ such that for $j \geq \tau\text{cap}(\mathbb{E})$

$$\Big|f_j - e^{\tau c}\frac{[\tau\text{cap}(\mathbb{E})]^j}{j!}\Big| \leq \frac{K}{\sqrt{j}}\frac{[\tau\text{cap}(\mathbb{E})]^j}{j!}, K_1\frac{[\tau\text{cap}(\mathbb{E})]^j}{j!} \leq \eta_j(G,\mathbb{D}) \leq K_2\frac{[\tau\text{cap}(E)]^j}{j!}.$$

Idea of proof: convexity plus "elementary" properties of ψ allows to show that

$$|\frac{\psi(Re^{it}) - \psi(R)}{\text{cap}(\mathbb{E})} - R(e^{it} - 1)| \leq \frac{|t|}{R} \quad \Longrightarrow$$

$$|e^{\tau(\psi(Re^{it}) - \psi(R))} - e^{\tau\text{cap}(\mathbb{E})R(e^{it}-1)}| \leq \frac{\tau\text{cap}(\mathbb{E})}{R}|t| \quad \Longrightarrow$$

$$\Big|e^{-\tau\psi(R)}f_j - \frac{1}{2\pi i}\int_{|u|=R}\frac{e^{\tau\text{cap}(\mathbb{E})(u-R)}}{u^{j+1}}du\Big| \leq \frac{1}{\pi}\int_0^{\pi}\frac{\tau\text{cap}(\mathbb{E})}{R}|t|\frac{dt}{R^j} = \frac{\pi}{2}\frac{\tau\text{cap}(\mathbb{E})}{R^{j+1}}$$

now take $R = \frac{j}{\tau\text{cap}(\mathbb{E})} \geq 1$. □

Can we do something for $j < \tau\text{cap}(\mathbb{E})$?

Sometimes one may exploit the trivial bound

$$|f_j| \leq \min_{R \geq 1} \frac{e^{\tau\psi(R)}}{R^j}$$

with minimum attained at $R = 1$ if $j < \tau\psi'(1)$ (notice that $\psi'(1) = 0$ if $\mathbb{E}$ has an outer angle $> \pi$ at $\psi(1)$), and else at $\widetilde{R}$ being unique solution of $\tau R\psi'(R) = j$.

Example (Hochbruck and Lubich): let $\mathbb{E} = [-4\rho, 0]$ then

$$\psi(w) = \text{cap}(\mathbb{E})(w + \frac{1}{w} - 2), \quad R\psi'(R) = \text{cap}(\mathbb{E})(R - \frac{1}{R}),$$

and thus for all $0 \leq j \leq \tau\text{cap}(\mathbb{E})$

$$|f_m| \leq \exp\Big(-\frac{j^2}{7\tau\text{cap}(\mathbb{E})}\Big), \qquad \eta_j(G, \mathbb{D}) \leq K_3 \exp\Big(-\frac{m^2}{7\tau\text{cap}(\mathbb{E})}\Big).$$

Application 2: powers/Markov functions

Consider $\mathbb{E} \supset W(A)$ symmetric with respect to real axis (e.g., $A \in \mathbb{R}^{d \times d}$), and

$$g(z) = \int_\alpha^\beta \frac{d\mu(t)}{z - t}, \quad \alpha < \beta < \gamma = \min\{\mathrm{Re}(z) : z \in \mathbb{E}\},\ \mu \geq 0.$$

Example: $z^\kappa = \frac{\sin(\pi|\kappa|)}{\pi} \int_{-\infty}^0 \frac{|t|^\kappa}{z-t} dt$ for $\kappa \in (-1, 0)$.

Here Faber coefficients $g_j = -\int_\alpha^\beta \phi(t)^{-j-1} \phi'(t) d\mu(t)$ with sign $(-1)^j$.

Improved: $\sum_{j=0}^\infty |g_{m+j(m+1)}| \leq \eta_m(G, \mathbb{D}) \leq \sum_{j=0}^\infty |g_{m+2j}|$ sharp up to $\frac{m+1}{2}$.

COROLLARY 5: For Markov function

$$\|g(A)b - V_m g(H_m) e_1\| \leq 4 \int_\alpha^\beta \frac{|\phi'(t)|}{|\phi(t)|^2 - 1} \frac{d\mu(t)}{|\phi(t)|^{m-1}} \leq 4 \frac{|g(\gamma)|}{|\phi(\gamma)|^m} = 4 \frac{\|g\|_{L_\infty(\mathbb{E})}}{|\phi(\gamma)|^m}.$$

A special case of Markov: FOM

Consider

$$x_m := V_m H_m^{-1} e_1 \in \mathsf{span}(V_m) = \mathsf{span}(b, Ab, ..., A^{m-1}b)$$

then

$$\begin{aligned} b - Ax_m &= b - (AV_m)H_m^{-1}e_1 = b - (V_m H_m + f_m e_m^*)H_m^{-1}e_1 \\ &= -f_m e_m^* H_m^{-1} e_1 \perp \mathsf{span}(V_m) = \mathsf{span}(b, Ab, ..., A^{m-1}b) \end{aligned}$$

i.e., x_m is FOM iterate. From previous slide for $0 \notin \mathbb{E} \supset W(A)$ symmetric with respect to real axis with $g(x) = 1/x$

$$\|A^{-1}b - x_m\| \leq \frac{4\,|\phi(0)|^{-m}}{\mathsf{dist}(0, \mathbb{E})}.$$

Closely related known estimate

$$\frac{\|A^{-1}b - x_m\|}{\|A^{-1}b\|} \leq \frac{\|A\|}{\mathsf{dist}(0, \mathbb{E})} \inf_{\deg q < m} \|A^{-1}b - q_{m-1}(A)b\|.$$

... some final comments ...

... and what to do with

$$\log(z) = (z-1)\int_{-\infty}^{0} \frac{1}{z-t}\frac{dt}{1-t},$$

$$z^{7/2} = z^4 z^{-1/2} = z^4 \int_{-\infty}^{0} \frac{1}{z-t}\frac{dt}{\pi\sqrt{|t|}},$$

... we go back to the proof of THM 2: if $\widetilde{g}(z) = p(z) + q(z)g(z)$ with $\deg q = s, \deg p \leq m+s-1$ and $G = \mathcal{F}(g)$ then

$$\|\widetilde{g}(A)b - V_{m+s}\widetilde{g}(H_{m+s})b\| \leq 4\|q(A)b\|\eta_m(G,\mathbb{D}).$$

Open: how to deal with ϕ_ℓ functions?