Field of value error bounds for approximating matrix functions via rational Arnoldi

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Outline

The problem: approximating $g(A)b$ for large sparse $A \in \mathbb{R}^{d\times d}$, $b \in \mathbb{R}^d$,
and, e.g., $g(z) = \exp(\tau z)$, $g(z) = \sqrt{z}$, $g(z) = \log(z)$

The method: (rational) Arnoldi

The aim: "simple" a priori error estimates in terms of
field of values $W(A) = \{y^* Ay : \|y\| = 1\}$

The question: link with best polynomial/rational approx. of g on $W(A)$?

The aim: Simple sharp explicit upper bounds

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The problem and some applications

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

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

Applications for $g(z) = e^z$, $g(z) = \cos(z)$, $g(z) = \sin(z)$: semi-discretized PDEs or ODEs.

Applications for $g(z) = 1/\sqrt{z}$: splitting techniques in implicit schemes, stochastic differential equations.

Applications for $g(z) = \log(z)$, $g(z) = \tanh(z)$, ...

...recent SIAM book of Nick Higham.

Approximating via the Arnoldi method

We compute ONB $V_m = (v_1, ..., v_m) \in \mathbb{C}^{d\times m}$ of $\text{span}(b, Ab, ..., A^{m-1}b)$ via

$$v_1 = b, \qquad h_{j+1,j}v_{j+1} = Av_j - h_{1,j}v_1 - ... - h_{j,j}v_j,$$

leading to Arnoldi decomposition

$$AV_m = V_m H_m + (0, ..., 0, h_{m+1,m}v_{m+1}), \quad H_m = V_m^* A V_m \text{ upper Hessenberg.}$$

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? For each polynomial p of degree $< m$ we have $p(A)b = p(A)V_m e_1 = V_m p(H_m) e_1$, and thus

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

Approximating via rational Arnoldi

Consider some fixed denominator polynomial $q(z) = (1 - z/z_1)...(1 - z/z_m)$.

Rough idea (following Ruhe):

we compute ONB $V_{m+1} = (v_1, ..., v_{m+1})$ of

$$q(A)^{-1}\text{span}(b, Ab, ..., A^m b) = \text{span}(b, (z_1 I - A)^{-1} b, ..., (z_m I - A)^{-1} b)$$

and then project:

$$A_{m+1} = V_{m+1}^* A V_{m+1}.$$

The rational Arnoldi approximation with fixed denominator q of $g(A)b$

$$V_{m+1} g(A_{m+1}) V_{m+1}^* b = V_{m+1} g(A_{m+1}) e_1$$

gives the exact answer for any rational function $g = p/q$ with $\deg p \leq m$.
Also, we recover ordinary Arnoldi with $A_{m+1} = H_{m+1}$ for
$z_1 = ... = z_m = \infty$.

Rational Arnoldi: some more details

For fixed denominator polynomial $q(z) = (1 - z/z_1)...(1 - z/z_m)$, take z_0 far from the other z_j, and put $z_{m+1} = \infty$.

We compute ONB $V_{m+1} = (v_1, ..., v_{m+1})$ of $q(A)^{-1}\text{span}(b, Ab, ..., A^m b)$ via

$$v_1 = b, \qquad h_{j+1,j}v_{j+1} = (z_j I - A)^{-1}(z_j - z_0)(A - z_0 I)v_j - h_{1,j}v_1 - ... - h_{j,j}v_j,$$

leading to a more complicated Arnoldi decomposition: with $D_{m+1} = \text{diag}\,(\frac{1}{z_1 - z_0}, ..., \frac{1}{z_{m+1} - z_0})$, and $H_{m+1} = (h_{j,k})_{j,k=1,...,m+1}$ upper Hessenberg, we get after some computations

$$(A - z_0 I)V_{m+1}(I + H_{m+1}D_{m+1}) = V_{m+1}H_{m+1} + (0, ..., 0, h_{m+2,m+1}v_{m+2}),$$

implying that $A_{m+1} := V_{m+1}^* A V_{m+1} = z_0 I + H_{m+1}(I + H_{m+1}D_{m+1})^{-1}$.

Structured matrices are helpful for solving shifted systems.
If no structure, take repeated poles ($\Longrightarrow$ few LU decompositions)

How to get error estimates?

In both cases the error is governed by $\|g(A) - p(A)\|$ or $\|g(A) - \frac{p}{q}(A)\|$ for arbitrary polynomials p of degree $\leq m$.

Link with

$$\eta_m^q(g, \mathbb{E}) = \min_{\deg p \leq m} \|g - \frac{p}{q}\|_{L_\infty(\mathbb{E})} \quad ???$$

For normal matrices: take the maximum on the (convex hull of) the spectrum, but in the general case?

Crouzeix 2006: There exists a universal constant $C \in [2, 11.5]$ such that for any matrix $B \in \mathbb{C}^{d \times d}$ and for any function f analytic in the field of values

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

there holds

$$\|f(B)\| \leq C \, \|f\|_{L_\infty(W(B))}.$$

In what follows let $\mathbb{E} \subset \mathbb{C}$ be some convex and compact set symmetric with respect to the real axis and containing the field of values.

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Riemann maps and Faber operators

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

Faber operator: bijection between G analytic in $\mathbb{D}$ and g analytic in $\mathbb{E}$

$$z \in \mathrm{Int}(\mathbb{E}) : \qquad g(z) = \mathcal{F}(G)(z) = \frac{1}{2\pi i} \int_{|w|=1} \frac{\psi'(w)}{\psi(w) - z} G(w)\, dw,$$

$$w \in \mathrm{Int}(\mathbb{D}) : \qquad G(w) = \mathcal{F}^{-1}(g)(w) = \frac{1}{2\pi i} \int_{|\zeta|=1} \frac{g(\psi(\zeta))}{\zeta - w}\, d\zeta.$$

Faber polynomial: $F_n(z) = \mathcal{F}(w^n)(z)$ polynomial of degree n, namely F_n polynomial part of ϕ^n.

$G(w) = \frac{a}{w - w_1}$ with $|w_1| > 1$, $\mathcal{F}(G)(z) = \frac{a\psi'(w_1)}{z - \psi(w_1)}$, similar for multiple poles.

Hence with $Q(w) = \prod_j (w - w_j)$, $q(z) = \prod_j (z - z_j)$, $z_j = \psi(w_j)$ (Ellacott '83):

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

Our a priori bound

THEOREM 1: Let $\mathbb{E}$ as before containing the field of values $W(A)$ and let $g = \mathcal{F}(G)$ be analytic on $\mathbb{E}$, then for the rational q-Arnoldi method

$$\|g(A)b - V_{m+1}g(A_{m+1})e_1\| \leq 4\,\eta_m^Q(G, \mathbb{D})$$

(put $q = Q = 1$ for classical Arnoldi).

Our proof is inspired from Crouzeix, Delyon, Badea, BB 02-07, in particular the CRAS '05 of BB: $\|F_n(A)\| \leq 2$.

Also, we use $W(A_{m+1}) \subset W(A)$.

Previous work of Eiermann (1993), Greenbaum (1997), ...

Idea of proof of Theorem 1

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

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

Hence

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

Arnoldi $\Longrightarrow$ best polynomial approximation on $\mathbb{D}$

The Faber coefficients are given by

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

In the polynomial case $q = Q = 1$, we have

LEMMA 2:

$$|g_m| \le \eta^1_{m-1}(G, \mathbb{D}) \le \sum_{j=0}^{\infty} |g_{m+j}|.$$

Knizhnerman '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.

Example: $g(z) = \exp(\tau z)$, $\tau > 0$: if $m \ge \tau \text{cap}(\mathbb{E})$ then both $|g_m|$ and $\eta_m(G, \mathbb{D})$ can be bounded above and below by constants times $(\tau \text{cap}(\mathbb{E}))^m/(m!)$ (as in the disk case).

In general, if G is analytic in $|w| \le R$ then $|g_m| \le R^{-m} \|G\|_{L_\infty(\{|w| \le R\})}$.

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In general, if G is analytic in $|w| \leq R$ then $|g_m| \leq R^{-m} \|G\|_{L_\infty(\{|w| \leq R\})}$.

Rational Arnoldi $\Longrightarrow$ best rational approximation on $\mathbb{D}$ with prescribed poles

Rational approximation (with fixed denominator) allows for a better rate of convergence for functions analytic in parts of the plane like

$$\frac{1}{\sqrt{z}} = \int_{-\infty}^{0} \frac{1}{z-t} \frac{dx}{\pi\sqrt{|x|}}, \qquad \frac{\log(z)}{z-1} = \int_{-\infty}^{0} \frac{1}{z-x} \frac{dx}{1+|x|},$$

$$z^{\kappa} = \frac{\sin(\pi|\kappa|)}{\pi} \int_{-\infty}^{0} \frac{|x|^{\kappa}}{z-x} dx, \qquad \kappa \in (-1, 0),$$

or more generally **MARKOV FUNCTIONS**

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

Notice: $G = \mathcal{F}^{-1} g$ is also Markov function with support $[\phi(\alpha), \phi(\beta)] \subset [-\infty, -1)$.

The special case of Markov functions

Suppose in what follows that w_j occur in conjugate pairs, and $w_j = \phi(z_j) \in (\phi(\alpha), \phi(\beta))$ have even multiplicities. Thus $B(w) := \prod_{j=1}^{m} \frac{1 - w\overline{w_j}}{w - w_j}$ is of unique sign and of modulus ≥ 1 in $[\phi(\alpha), \phi(\beta)]$.

THEOREM 3: Under the above assumptions for $\mathbb{E}$, w_j, g

$$\int \frac{\phi'(x)}{|\phi(x)|^2 - 1/|B(\phi(x))|} \frac{d\mu(x)}{|B(\phi(x))|} \leq \eta_m^Q(G, \mathbb{D})$$

$$\leq \int \frac{\phi'(x)}{|\phi(x)|^2 - 1} \frac{d\mu(x)}{|B(\phi(x))|} \leq \|g\|_{L_\infty(\mathbb{E})} \max_{y \in [\phi(\alpha), \phi(\beta)]} \frac{1}{|yB(y)|}.$$

NB1: lower/upper bound differ by constant $1 - |\phi(\beta)|^{-2}$.

NB2: upper bound remains valid without assumptions on multiplicities.

Ideas of proof: for upper bound construct modified interpolant at $1/\overline{w}_j$ and 0. For lower bound compute explicitly best rational approximant on discrete subset of $\partial\mathbb{D}$.

How to choose the poles?

We have so far for Markov functions g

$$\|g(A)b - V_{m+1}g(A_{m+1})e_1\| \leq \frac{4\|g\|_{L_\infty(\mathbb{E})}}{|\phi(\beta)|} \max_{w\in[\phi(\alpha),\phi(\beta)]} \frac{1}{|B(w)|}, \qquad B(w) := \prod_{j=1}^{m} \frac{1 - w\overline{w_j}}{w - w_j}.$$

Choice of poles $z_j = \psi(w_j)$ by minimizing $1/B$ on $[\phi(\alpha), \phi(\beta)]$?

- one pole of multiplicity m.
- two poles of multiplicity $m/2$.
- k poles of multiplicity p, $m = pk$.

How to choose a single pole?

Let m be even. The problem

$$\min_{w_1 \in \mathbb{C}} \max_{[\phi(\alpha),\phi(\beta)]} \left| \frac{1 - \overline{w}_1 w}{w - w_1} \right|$$

can be solved explicitly with optimal pole

$$w_1 = w_{opt} = \frac{\widetilde{\phi}(\beta)\widetilde{\phi}(\alpha) + 1}{\widetilde{\phi}(\beta)\widetilde{\phi}(\alpha) - 1}, \qquad \widetilde{\phi}(w) = \sqrt{\frac{|\phi(w)| - 1}{|\phi(w)| + 1}} \in (0,1),$$

leading to the convergence rate

$$\max_{w \in [\phi(\alpha),\phi(\beta)]} \left| \frac{1 - \overline{w}_1 w}{w - w_1} \right|^m = \left(\frac{1 - \widetilde{\phi}(\beta)/\widetilde{\phi}(\alpha)}{1 + \widetilde{\phi}(\beta)/\widetilde{\phi}(\alpha)} \right)^m .$$

Example: if $[\alpha,\beta] = [-\infty, 0], \mathbb{E} = [\lambda_{\min}, \lambda_{\max}]$ then rate $\approx e^{-2m/\sqrt[4]{\kappa}}$, $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$.

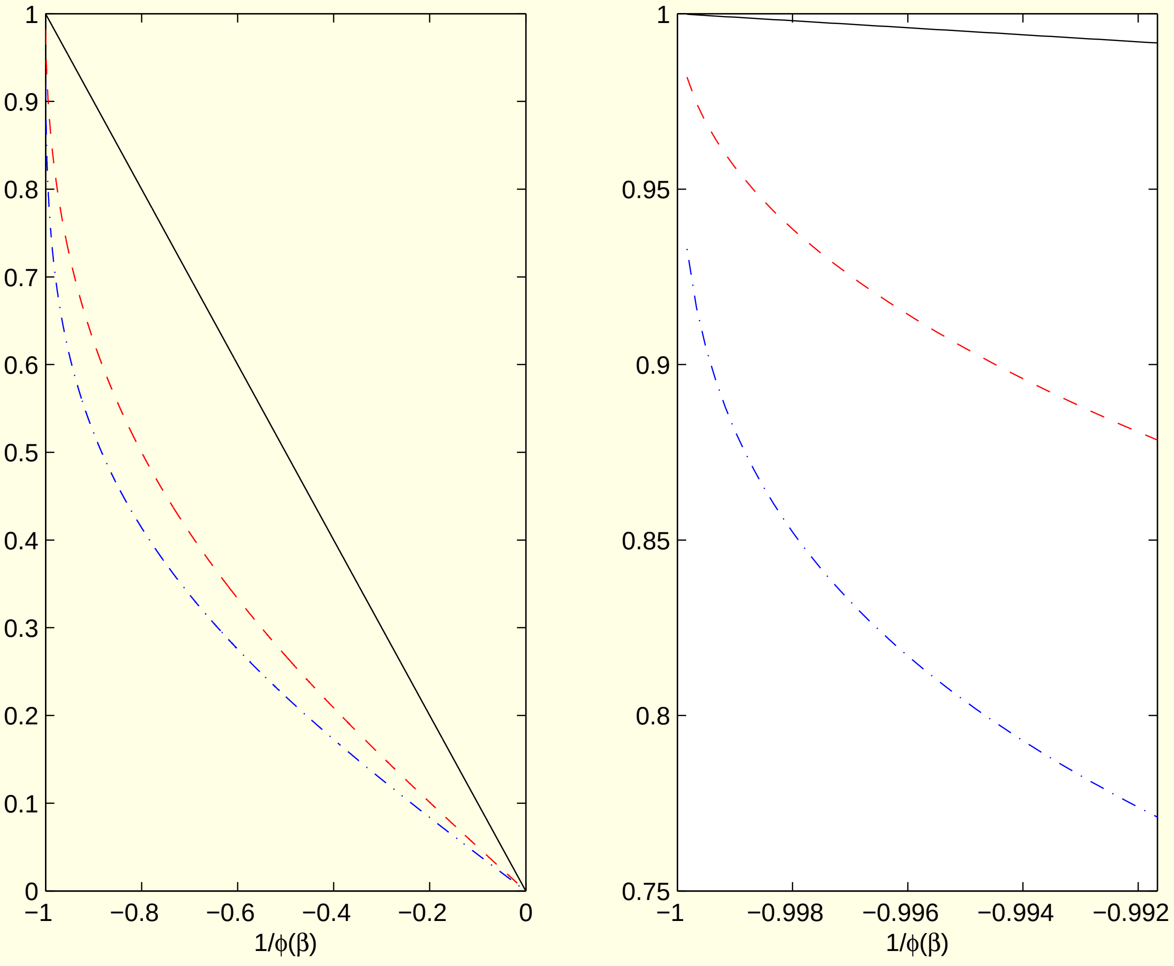
How to choose one finite pole?

We obtain exactly the same rate for a single pole as if we take the two poles $w_1 = \phi(\alpha)$ and $w_2 = \phi(\beta)$ with multiplicities $m/2$!

Special case $\alpha = \infty = w_1$: see Druskin & Knizhnerman '98 for symmetric A and Knizhnerman & Simoncini '08 for general A.

But we get a better rate c^m for $w_1 = \infty$ if we put the finite pole at $w_2 = -\frac{c^2+1}{2c}$, where c unique solution in $(0, 1/|\phi(\beta)|)$ of

$$-\sqrt{\frac{2c^2}{1+c^4}} = \frac{1/\phi(\beta)+c}{1+c/\phi(\beta)}.$$



How to choose real poles?

Let $m = pk$ for some integers $p, k \geq 1$.

This pole placement problem is reduced to the (classical) third Zolotarev problem for minimal Blaschke products on intervals $I \subset \mathbb{R} \setminus \mathbb{D}$:

find $Z_{k,I}$ the minimum $L_\infty(I)$ norm of a Blaschke product of order k,

the required poles $w_1, ..., w_k$ (repeated periodically) being the zeros of such a minimal Blaschke product $B_{k,I}$.

It is known that $R(I, \mathbb{D})^{-k} \leq Z_{k,I} \leq 2R(I, \mathbb{D})^{-k}$, and that for $j = 1, 2, ..., k$

$$w_j = \chi_{I,\mathbb{D}}\Big(\exp(2\pi i \frac{2j-1}{4k})\Big)$$

where $R(I, \mathbb{D})$ is the ring modulus and $\chi_{I,\mathbb{D}}$ the conformal map from $1 < |\zeta| < R$ onto the doubly connected set $\overline{C} \setminus (\mathbb{D} \cup I)$....

Convergence rate for k LU decompositions:

$$\max_{w \in [\phi(\alpha), \phi(\beta)]} 1/|B(w)| \leq 2^p R([\phi(\alpha), \phi(\beta)], \mathbb{D})^{-m}.$$

... 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 can go back to the proof of THM 1: if $\widetilde{g}(z) = p_1(z) + p_2(z)g(z)$ with $\deg p_2 = s, \deg p_1 \leq m+s$ and $G = \mathcal{F}(g)$ then with $z_{m+1} = ... = z_{m+s+1} = \infty$

$$\|\widetilde{g}(A)b - V_{m+s+1}\widetilde{g}(A_{m+s+1})e_1\| \leq 4\,\|p_2(A)b\|\,\eta_m^Q(G,\mathbb{D}).$$