Matrix functions and large-scale matrix equations: effective numerical solution strategies

V. Simoncini

Dipartimento di Matematica, Università di Bologna

valeria@dm.unibo.it

The Problem

Given $v \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n\times n}$, approximate

$$x = f(A)\, v$$

with f regular function such that $f(A)$ is well defined

Focus:

- A large dimension
- A symmetric pos. (semi)def., or A *positive real*

Context

- A of small dimension:

$$A \text{ symmetric}, \qquad A = X\Lambda X^\top \Rightarrow f(A) = Xf(\Lambda)X^\top$$

Similar, but more involved, the definition for A nonsymmetric

- A medium to large dimension:

$$f(A) \qquad \text{vs.} \qquad f(A)v$$

Applications

Among which:

- Numerical solution of evolution PDEs
  (e.g. $\exp(\lambda), \sqrt{\lambda^{-1}}, \cos(\lambda), \varphi_k(\lambda) ...$)
- Numerical solution of some Inverse Problems $(\exp(\lambda), \cosh(\lambda), ...)$
- Fluxes on manifolds
- Scientific Computing problems (e.g. QCD, $\mathrm{sign}(\lambda)$)
- (Analysis of) reduced Dynamical System Models
  (through Grammian Matrices)

Numerical approximation. I

$$f(A)v \quad \approx \quad \widetilde{x} \qquad \widetilde{x} = ???$$

Two wide paths:

- Substitute f with "simpler" function, $f \approx \mathcal{R}$

$$\|f(A)v - \widetilde{x}\| \le \|f(A)v - \mathcal{R}(A)v\| + \|\mathcal{R}(A)v - \widetilde{x}\|$$

and $\quad \Rightarrow \quad \widetilde{x} \approx \mathcal{R}(A)v$

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- Approximation by projection: Find V and

$$\widetilde{x} \in \mathrm{range}(V), \quad \mathrm{space\,dim} \ll n$$

Numerical approximation. II

$$f(A)v \quad \approx \quad \widetilde{x}$$

Important issues:

- $\star$ Measure accuracy of approximation?
- $\star$ Relation between f and quality of approximation
- $\star$ Relation between A and quality of approximation
- $\star$ Efficiency ?

Rational Approximation

$$x = f(A)\,v \quad \approx \quad \mathcal{R}_{\mu,\nu}(A)v$$

$$\mathcal{R}_{\mu,\nu}(\lambda) = \frac{\Phi_\mu(\lambda)}{\Psi_\nu(\lambda)}, \qquad \Phi_\mu(\lambda),\ \Psi_\nu(\lambda) \quad \text{polynomials}$$

- Polynomial Approx., $\nu = 0$
- Rational Approx.: Padé or Chebyshev, e.g. $\mu = \nu$
- Rational Approx with multiple pole
- Quadrature Methods

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We consider the case of partial fraction expansion:

$$\mathcal{R}_{\mu,\nu}(\lambda) = q(\lambda) + \sum_{k=1}^{\nu} \frac{\omega_k}{\lambda - \xi_k} \qquad (\mathcal{R}_\nu = \mathcal{R}_{\nu,\nu})$$

Rational Approximation: poles

$f(\lambda) = \exp(-\lambda)$

$\mathcal{R}_\nu$: ℓ_∞ best approx

in $[0, \infty)$, Chebyshev

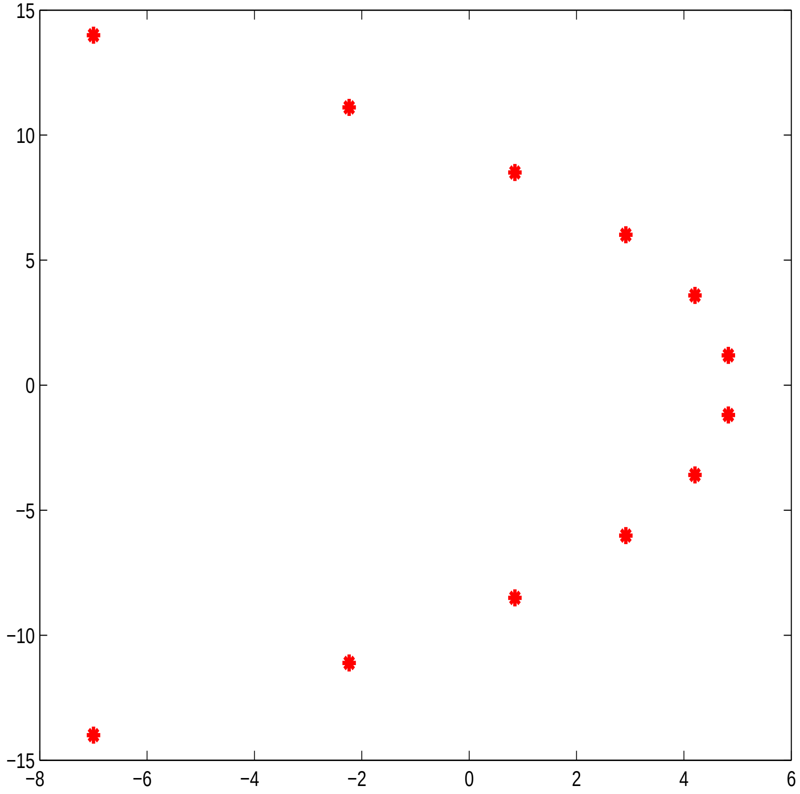
$\|f - \mathcal{R}_\nu\|_\infty \approx 10^{-\nu}$

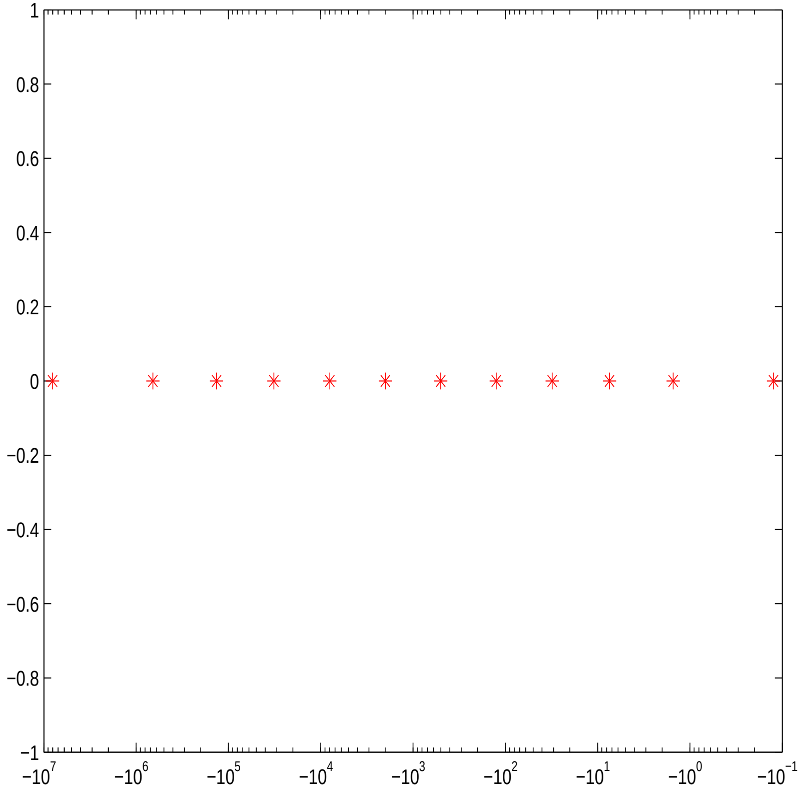
$f(\lambda) = \lambda^{-\frac{1}{2}}$

$\mathcal{R}_\nu$: Zolotarev approx

in $[a, b] \subseteq (0, \infty)$

$\|f - \mathcal{R}_\nu\| \approx e^{-\pi\sqrt{2\nu}}$





Matrix Rational approximation

$$
\begin{aligned}
f(A)v \quad \approx \quad \mathcal{R}_\nu(A)v &= \sum_{k=1}^{\nu} \omega_k (A - \xi_k I)^{-1} v \\
&\approx \sum_{k=1}^{\nu} \omega_k \widetilde{x}_k
\end{aligned}
$$

- $\forall k$, $(A - \xi_k I)$ "Shifted" matrix , $\xi_k \in \mathbb{C}$
- $\xi_{2j-1} = \bar{\xi}_{2j}$, $j = 1, \ldots, \lfloor \nu/2 \rfloor$
- $\forall k$, $\widetilde{x}_k$ approx solution

Matrix Rational approximation

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$\Rightarrow$ Iterative Methods for **shifted** linear systems

Error estimates

$\widetilde{x}_k$: Krylov subspace methods: $\sum_{k=1}^{\nu} \omega_k (A - \xi_k I)^{-1} v \approx \sum_{k=1}^{\nu} \omega_k \widetilde{x}_k$

$$\|\mathcal{R}_\nu(A)v - \sum_{k=1}^{\nu} \omega_k \widetilde{x}_k\| =??$$

Error estimate during iteration : (Frommer & S., '08)

- Estimate for real symmetric A and complex poles
- Lower estimate for A spd and real negative poles

Error estimates

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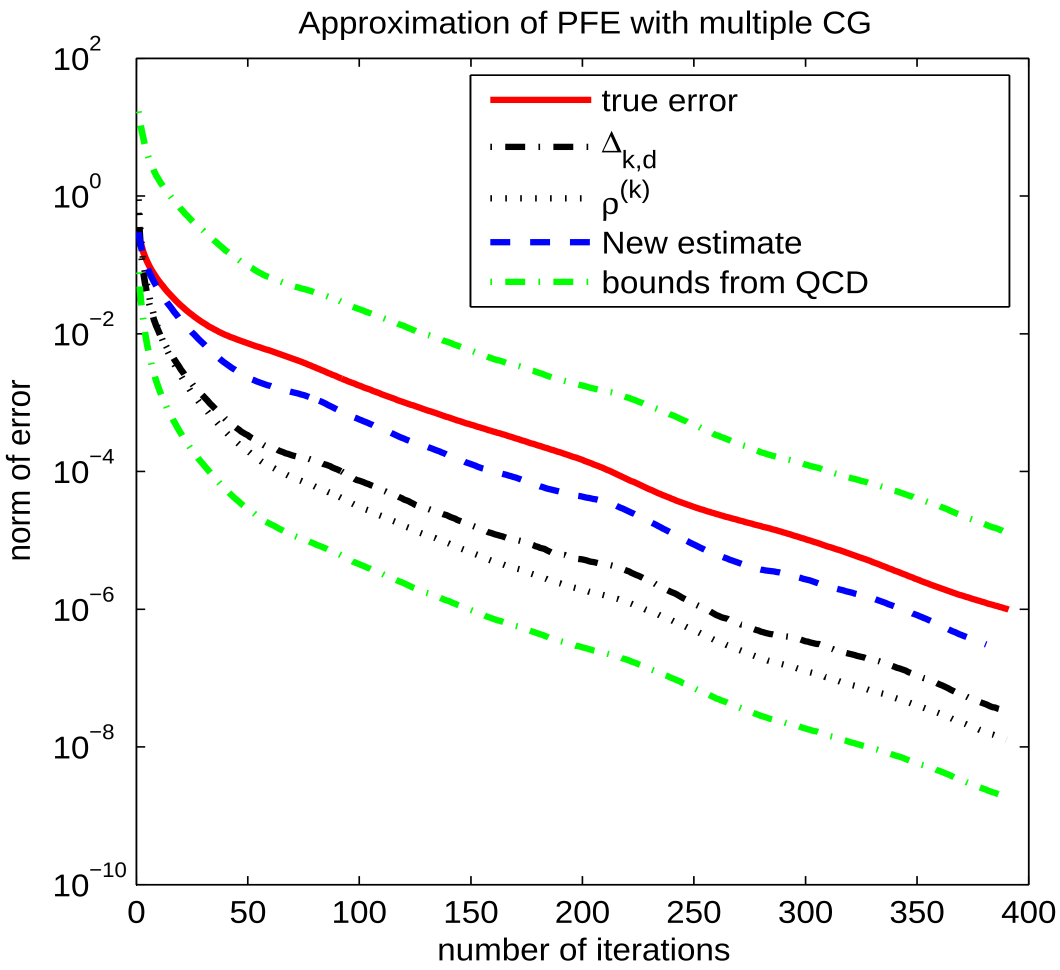
Error estimate during iteration : (Frommer & S., '08)

- Estimate for real symmetric A and complex poles
- Lower estimate for A spd and real negative poles

⋆ Does not require spectral info

⋆ Computational cost only 3-5 additional iterations

CG for A spd and $f(\lambda) = \mathrm{sign}(\lambda) = (\lambda^2)^{-\frac{1}{2}}\lambda :\quad \mathrm{sign}(A)v$



Projection-type methods

$\mathcal{K}$ approximation space, $m = \dim(\mathcal{K})$

$V \in \mathbb{R}^{n\times m}$ s.t. $\mathcal{K} = \text{range}(V)$

$$x = f(A)v \quad \approx \quad x_m = Vf(V^\top AV)(V^\top v)$$

Question: Which $\mathcal{K}$?

Some explored alternatives for $\mathcal{K}$

- Krylov subspace, $\mathcal{K} = K_m(A, v)$
- Shift-Invert Krylov subspace, $\mathcal{K} = K_m((I + \gamma A)^{-1}, v)$ for some γ
- Rational Krylov subspace, for some $\omega_1, \omega_2, \ldots$

$$\mathcal{K} = \text{span}\{v, (A - \omega_1 I)^{-1} v, (A - \omega_2 I)^{-1} v, \ldots\}$$

- Extended Krylov subspace, $\mathcal{K} = K_m(A, v) + K_m(A^{-1}, A^{-1} v)$
- Restarted Krylov subspace

Note: In all cases, A nonsymmetric.

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Theory mostly for field of values of A in $\mathbb{C}^+$

Field of values: $W(A) = \{x^* A x,\ x \in \mathbb{C}^n, \|x\| = 1\}$

Krylov subspace approximation

"Classical" approach:

$$\mathcal{K} = K_m(A, v) = \text{span}\{v, Av, \ldots, A^{m-1}v\}$$

For $H_m = V_m^\top A V_m$, $v = V_m e_1$ and $V_m^\top V_m = I_m$:

$$x_m = V_m f(H_m) e_1$$

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Polynomial approximation: $x_m = p_{m-1}(A)v$
(p_{m-1} interpolates f at eigenvalues of H_m)

⋆ Numerical and theoretical results since mid '80s
(van der Vorst'87, Saad'92, Hochbruck & Lubich'97, ..., Beckermann& Reichel'10)

Application. Evolution Problem

$$\begin{cases} \frac{\partial u(x,y,t)}{\partial t} = \Delta u, \quad (x,y) \in (0,1)^2 \quad t \in [0, 0.1] \\ u(x,y,t) = 0, \quad (x,y) \in \partial([0,1]^2) \\ u(x,y,0) = 1, \quad (x,y) \in [0,1]^2 \end{cases}$$

Implicit Euler: $u_{i+1} = (I + \delta t A)^{-1} u_i, \quad i = 0, 1, ...$

Exponential Integrator: $u(t) = \exp(-tA) u_0 \quad t = 0.1$

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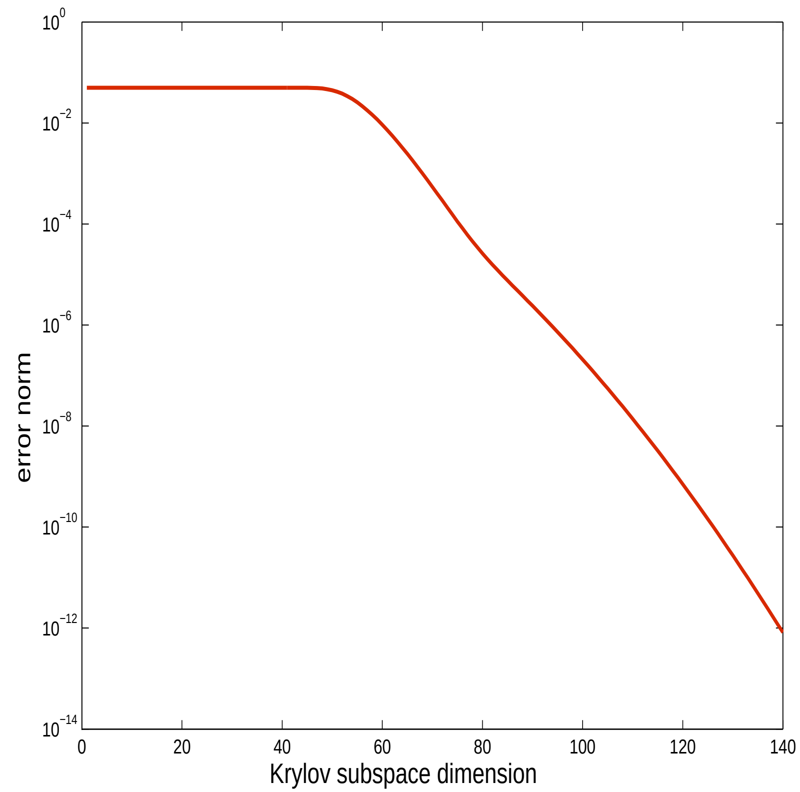
	Euler		Exp	
step δt	CPU	error	CPU	error (#its*)
0.001	1.9	$2 \cdot 10^{-3}$	0.09	$9 \cdot 10^{-4}$(37)
0.005	0.4	$1 \cdot 10^{-2}$	0.07	$4 \cdot 10^{-3}$(28)
0.01	0.2	$2 \cdot 10^{-2}$	0.05	$1 \cdot 10^{-2}$(25)

* : Stopping criterion tolerance related to Euler timestep

$\Rightarrow$ More general exponential integrators (see Hochbruck's talk)

...When things are not so easy

$$\|\exp(-A)v - V_m \exp(-H_m)e_1\| \qquad A \in \mathbb{R}^{400\times 400}, \|A\| = 10^5$$



$$\|\exp(-A)v - V_m \exp(-H_m)e_1\| \leq 10e^{-m^2/(5\rho)}, \qquad \sqrt{4\rho} \leq m \leq 2\rho$$

where $\sigma(A) \subseteq [0, 4\rho]$

Acceleration Procedures: Shift-Invert Krylov

Choose γ s.t. $(I + \gamma A)$ is invertible, and construct

$\mathcal{K} = K_m((I + \gamma A)^{-1}, v)$, Moret-Novati '04, van den Eshof-Hochbruck '06

with $T_m = V_m^\top (I + \gamma A)^{-1} V_m$, $v = V_m e_1$ and $V_m^\top V_m = I_m$

$$x_m = V_m f(\frac{1}{\gamma}(T_m^{-1} - I_m))e_1$$

Rational approximation: $x_m = p_{m-1}((I + \gamma A)^{-1})v$

Choice of γ: A spd, $\gamma = \frac{1}{\sqrt{\lambda_{\min}\lambda_{\max}}}$ (Moret, '09)

A nonsym, (Beckermann & Reichel'10)

Acceleration Procedures: Extended Krylov

For A nonsingular,

$\mathcal{K} = K_{m_1}(A, v) + K_{m_2}(A^{-1}, A^{-1}v),$ Druskin & Knizhnerman'98, A sym.

Note: $\mathcal{K} = A^{-m_2} K_{m_1+m_2}(A, v)$

Algorithm (augmentation-style)

- Fix $m_2 \ll m_1$
- Run m_2 steps of Inverted Lanczos
- Run m_1 steps of Standard Lanczos + orth.

Extended Krylov: an effective implementation

$m_1 = m_2 = m$ not fixed a priori

$$\begin{aligned} \mathcal{K} &= K_m(A, v) + K_m(A^{-1}, A^{-1}v) \\ &= \text{span}\{v, A^{-1}v, Av, A^{-2}v, A^2v, \ldots\} \end{aligned}$$

⋆ *Block* Arnoldi-type recurrence:

- $U_1 \leftarrow \text{orth}([v, A^{-1}v])$
- $U_{j+1} \leftarrow [AU_j(:,1), A^{-1}U_j(:,2)]$ + orth $\quad j = 1, 2, \ldots$

⋆ Recurrence to cheaply compute $\mathcal{T}_m = \mathcal{U}_m^\top A \mathcal{U}_m, \quad \mathcal{U}_m = [U_1, \ldots, U_m]$

⋆ Compute $x_m = \mathcal{U}_m f(\mathcal{T}_m) e_1$

Simoncini '07

Extended Krylov: Convergence theory I

f satisfying $\quad f(z) = \int_{-\infty}^{0} \frac{1}{z-\zeta} d\mu(\zeta), \quad z \in \mathbb{C}\backslash]-\infty, 0]$

(with convenient measure $d\mu(\zeta)$)

Extended Krylov: Convergence theory II

Nonsingular A, with $0 \notin W(A)$.

Let Φ_1, Φ_2 be the conformal mappings for $W(A)$ and $W(A)^{-1}$

There exists $a > 0$ s.t. $|\Phi_1(-a)| = |\Phi_2(-\frac{1}{a})|$ so that

$$\| f(A)v - \mathcal{U}_m f(\mathcal{T}_m)e_1 \| \le \frac{c}{|\Phi_1(-a)|^m}$$

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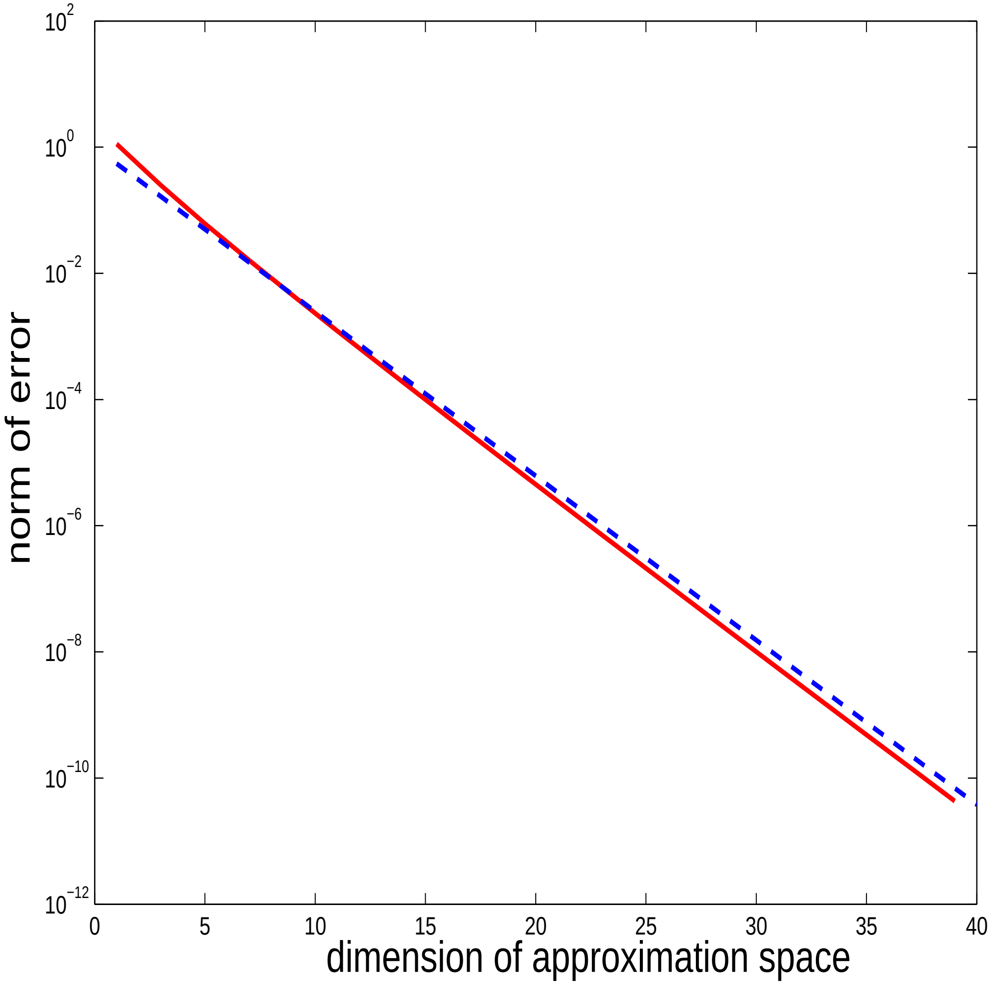
e.g. for A symmetric (Φ_1, Φ_2 known, $a = \sqrt{\lambda_{\min}\lambda_{\max}}$) :

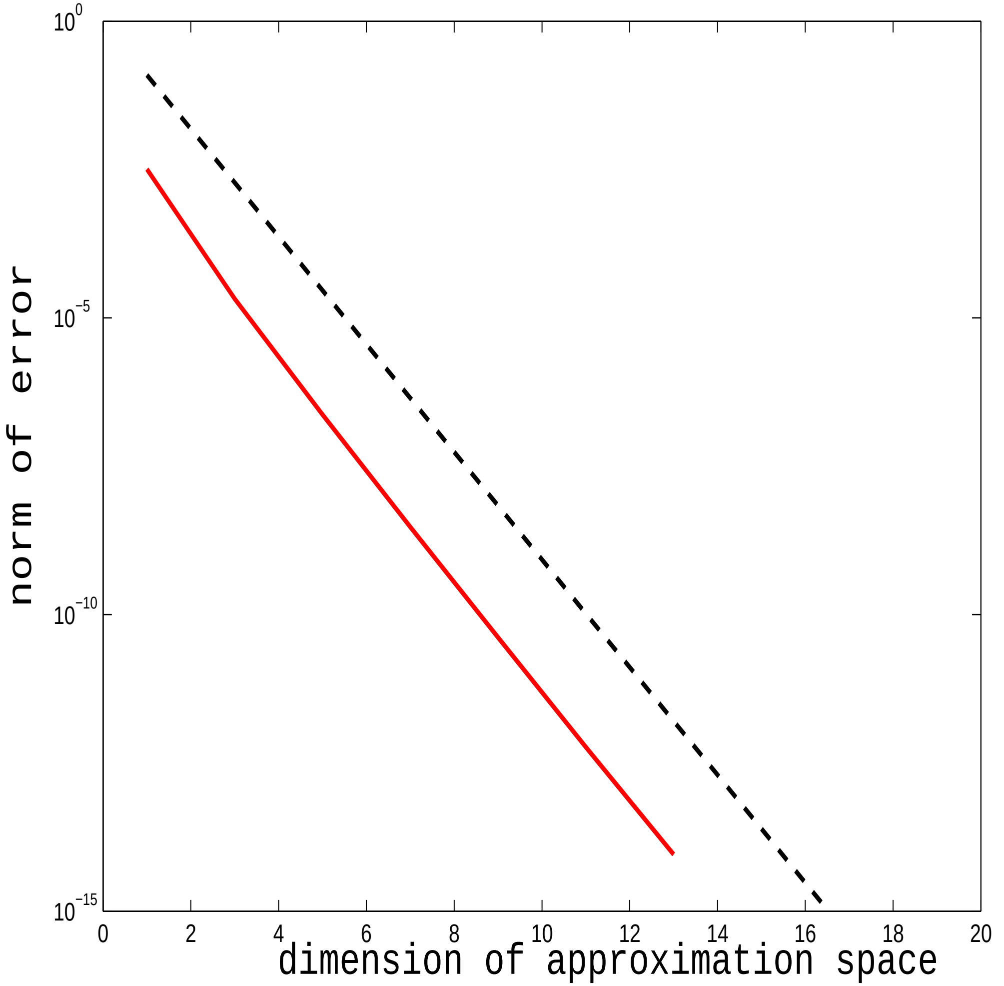
$\|x - x_m\| = O(\exp(-2m\sqrt[4]{\frac{\lambda_{\min}}{\lambda_{\max}}}))$

Convergence rate. $A \in \mathbb{R}^{400\times 400}$ normal. $f(\lambda) = \lambda^{-\frac{1}{2}}$



$\sigma(A)$ on an elliptic curve in $\mathbb{C}^+$ with center on real axis

Rate. $A \in \mathbb{R}^{200\times 200}$ Jordan block, $\sigma(A) = \{4\}$. $f(\lambda) = \lambda^{\frac{1}{2}}$



$W(A)$ disk centered at 4 and unit radius

Large-scale numerical experiments

A from FD discretization of

$$\begin{aligned}
\mathcal{L}_1(u) &= -100u_{x_1x_1} - u_{x_2x_2} + 10x_1u_{x_1}, \\
\mathcal{L}_2(u) &= -100u_{x_1x_1} - u_{x_2x_2} - u_{x_3x_3} + 10x_1u_{x_1}, \\
\mathcal{L}_3(u) &= -e^{-x_1x_2}u_{x_1x_1} - e^{x_1x_2}u_{x_2x_2} + \frac{1}{x_1+x_2}u_{x_1}, \\
\mathcal{L}_4(u) &= -\mathrm{div}(e^{3x_1x_2}\mathrm{grad}u) + \frac{1}{x_1+x_2}u_{x_1}
\end{aligned}$$

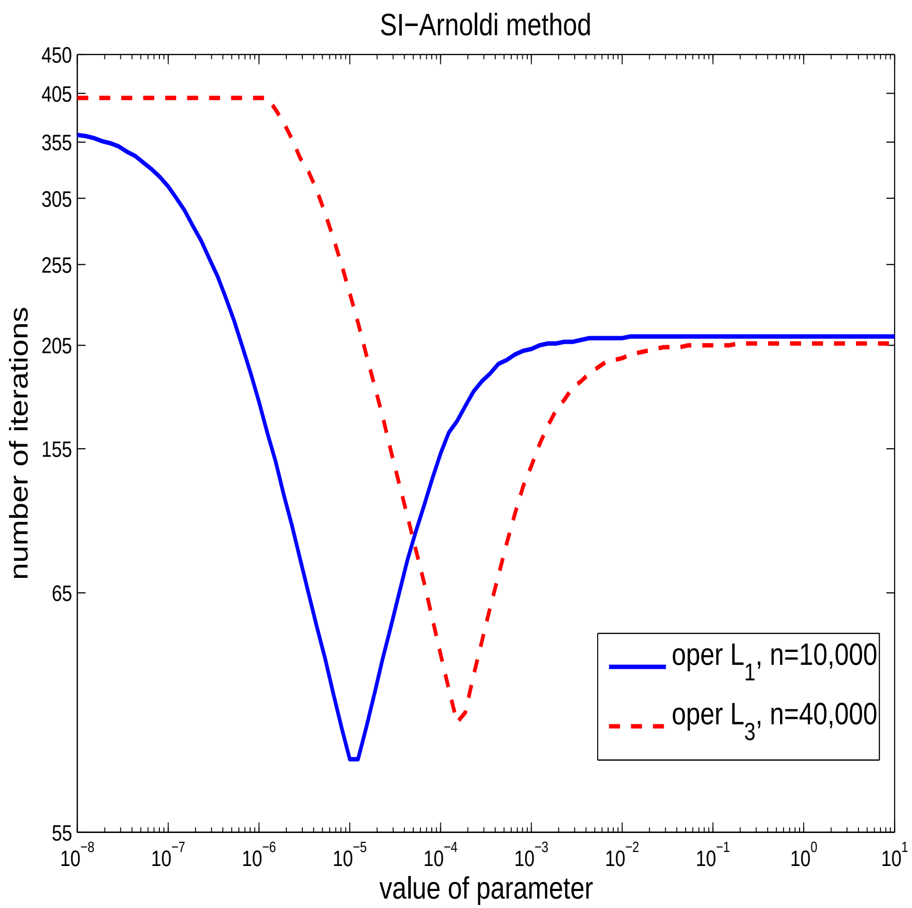
on unit square/cube, Dirichlet hom. bc.

Inner system solves:

- Extended Krylov: systems with A solved with GMRES/AMG
- SI-Arnoldi: span$\{v, (I+\gamma A)^{-1}v, (I+\gamma A)^{-2}v, \ldots\}$
  systems with $I + \gamma A$ solved with IDR(s)/ILU

An intermezzo

SI-Arnoldi requires getting the parameter γ:



Number of SI-Arnoldi iterations as a function of the parameter for $f(\lambda) = \lambda^{\frac{1}{2}}$

Comparisons: CPU Time in Matlab (space dim.)

f	Oper.	n	SI-Arnoldi	EKSM	Std Krylov
$\lambda^{\frac{1}{2}}$	$\mathcal{L}_1$	2500	0.9 (*59*)	0.6 (*48*)	7 (*193*)
		10000	4.0 (*66*)	3.6 (*68*)	*46 (*300*)
		160000	642.9(*246*)	219.7(*122*)	*458(*300*)
	$\mathcal{L}_2$	27000	10.8 (*55*)	7.4 (*40*)	6.7(*119*)
		125000	86.7 (*60*)	65.3 (*52*)	138.7(*196*)
	$\mathcal{L}_3$	40000	26.3 (*75*)	21.1 (*72*)	*87 (*300*)
		160000	318.5(*144*)	173.3 (*96*)	*442(*300*)
	$\mathcal{L}_4$	40000	41.1(*117*)	25.4(*106*)	*89 (*300*)
		160000	580.2(*442*)	231.2(*144*)	*461 (*300*)

Comparisons: CPU Time in Matlab (space dim.)

f	Oper.	n	SI-Arnoldi	EKSM	Std Krylov
$\lambda^{-\frac{1}{3}}$	$\mathcal{L}_1$	2500	0.6 (*43*)	0.4 (*30*)	2.2(*131*)
		10000	2.6 (*46*)	1.8 (*38*)	26.2(*252*)
		160000	79.3 (*48*)	99.7 (*64*)	*460(*300*)
	$\mathcal{L}_2$	27000	7.8 (*41*)	4.8 (*26*)	3.1 (*82*)
		125000	64.8 (*45*)	38.9 (*32*)	67.5(*138*)
	$\mathcal{L}_3$	40000	20.7 (*61*)	13.7 (*48*)	*88 (*300*)
		160000	116.5 (*62*)	105.2 (*62*)	*460 (*300*)
	$\mathcal{L}_4$	40000	35.8(*104*)	14.2 (*66*)	*88 (*300*)
		160000	208.1(*104*)	112.2 (*84*)	*461 (*300*)

Stopping criterion

Unlike linear systems: no equation $\Rightarrow$ no residual

Estimate of the error:

(first suggested for $f(\lambda) = e^{-\lambda}$ by van den Eshof-Hochbruck '06)

$$\frac{\|x - x_m\|}{\|x_m\|} \approx \frac{\delta_{m+j}}{1 - \delta_{m+j}}, \qquad \delta_{m+j} = \frac{\|x_{m+j} - x_m\|}{\|x_m\|}$$

Stopping criterion:

$$\texttt{if } \frac{\delta_{m+j}}{1-\delta_{m+j}} \leq \texttt{ tol then stop}$$

Computational costs awareness: inexact solves in EKSM

systems with A: GMRES with relaxed inner tolerance

$$\epsilon_m^{(\mathrm{inner})} = \frac{\texttt{tolin}}{\|x - x_{m-1}\|}.$$

Final outer error (# outer its / # inner its)

`tolin`	fixed inner tol	relaxed inner tol
1e-10	6.97e-11 (24/901)	6.58e-11 (24/559)
1e-12	6.48e-11 (24/1052)	6.48e-11 (24/716)

$\mathcal{L}(u) = -u_{xx} - u_{yy} - u_{zz} + 50(x+y)u_x$

$f(\lambda) = \lambda^{-\frac{1}{3}}$ $\qquad \epsilon^{(\mathrm{outer})} = 10^{-10}$

References

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