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Numerical Approximation of Matrix Functions and Applications

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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)

$\Rightarrow$ Some examples later on.

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⇒ Some examples later on. The idea:

$$\begin{cases} y' = -Ay \\ y(0) = y_0 \end{cases} \quad \Rightarrow \quad y(t) = \exp(-tA)y_0$$

Numerical approximation. I

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

Various alternatives. Among which:

- Substitute f with "simpler" function, $f \approx \mathcal{R}$
  for instance, $\mathcal{R}$ rational function:

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

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

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- Approximation by projection: Find V and

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

Numerical approximation. II

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

The important issues:

- $\star$ Measures for goodness 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., $\nu = 0$

  (Druskin & Knizhnerman, '89, Bergamaschi & Vianello, '00)

- Rational Approx.: Padé or Chebyshev, e.g. $\mu = \nu$
- Rational Approx with multiple pole
- Quadrature Methods (Trefethen etal.)

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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

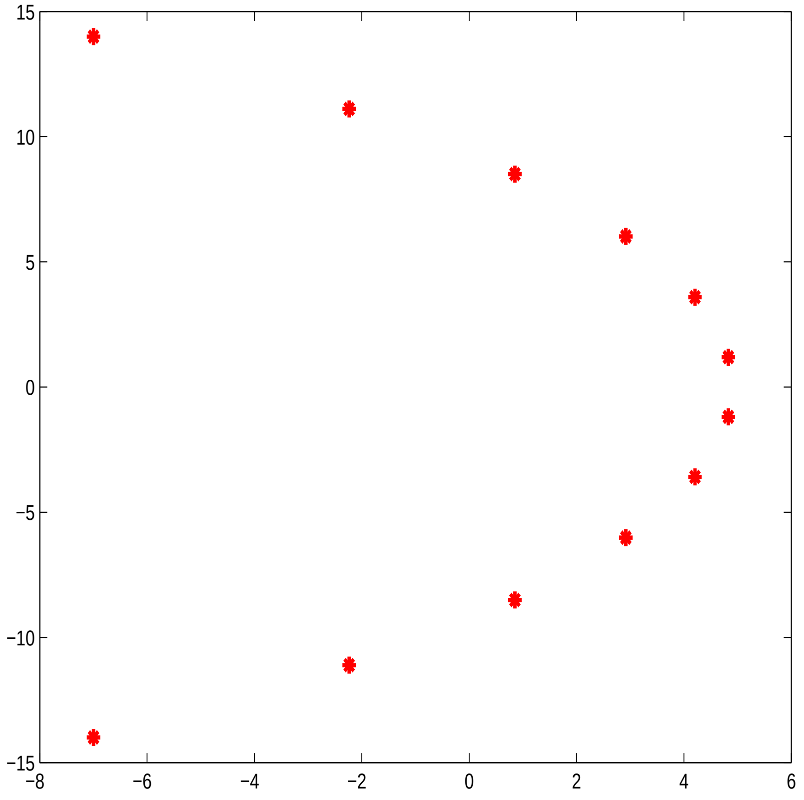
$\|f - \mathcal{R}_\nu\|_\infty \approx 10^{-\nu}$

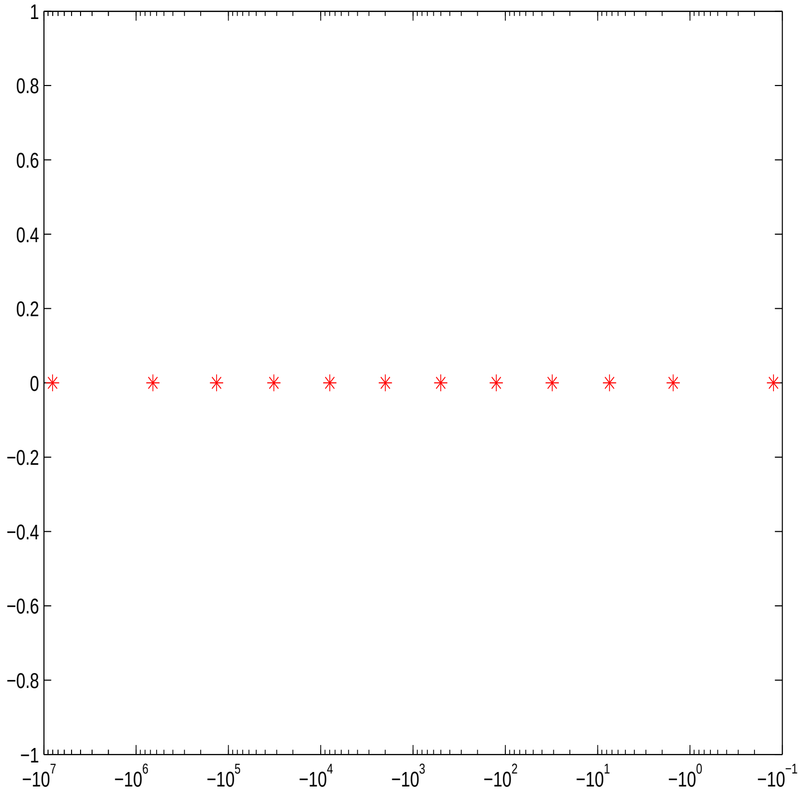
$f(\lambda) = \lambda^{-1/2}$

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

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

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





Matrix Rational approximation

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

- $\forall k$, $(A - \xi_k I)$ "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

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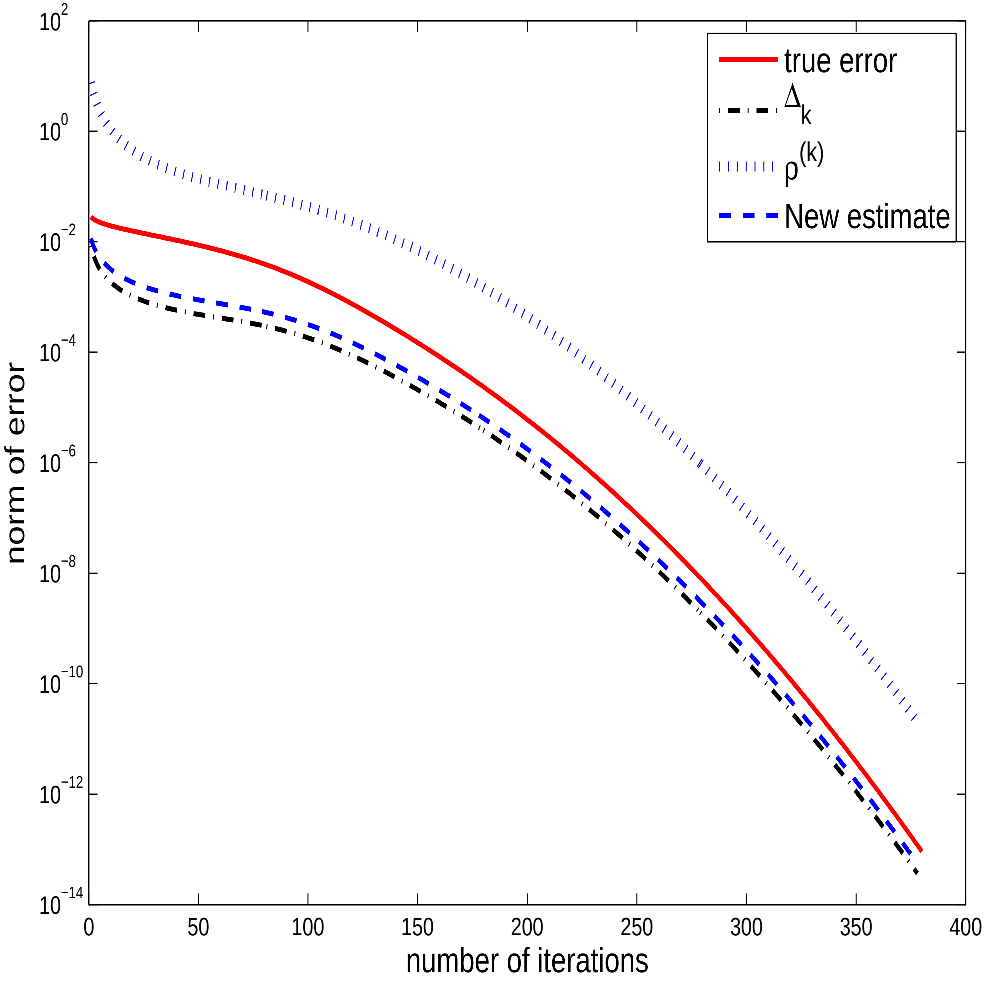
- Estimate for real symmetric A and complex poles
- Lower estimate for A spd and real negative poles

Estimate:

⋆ Does not require spectral info

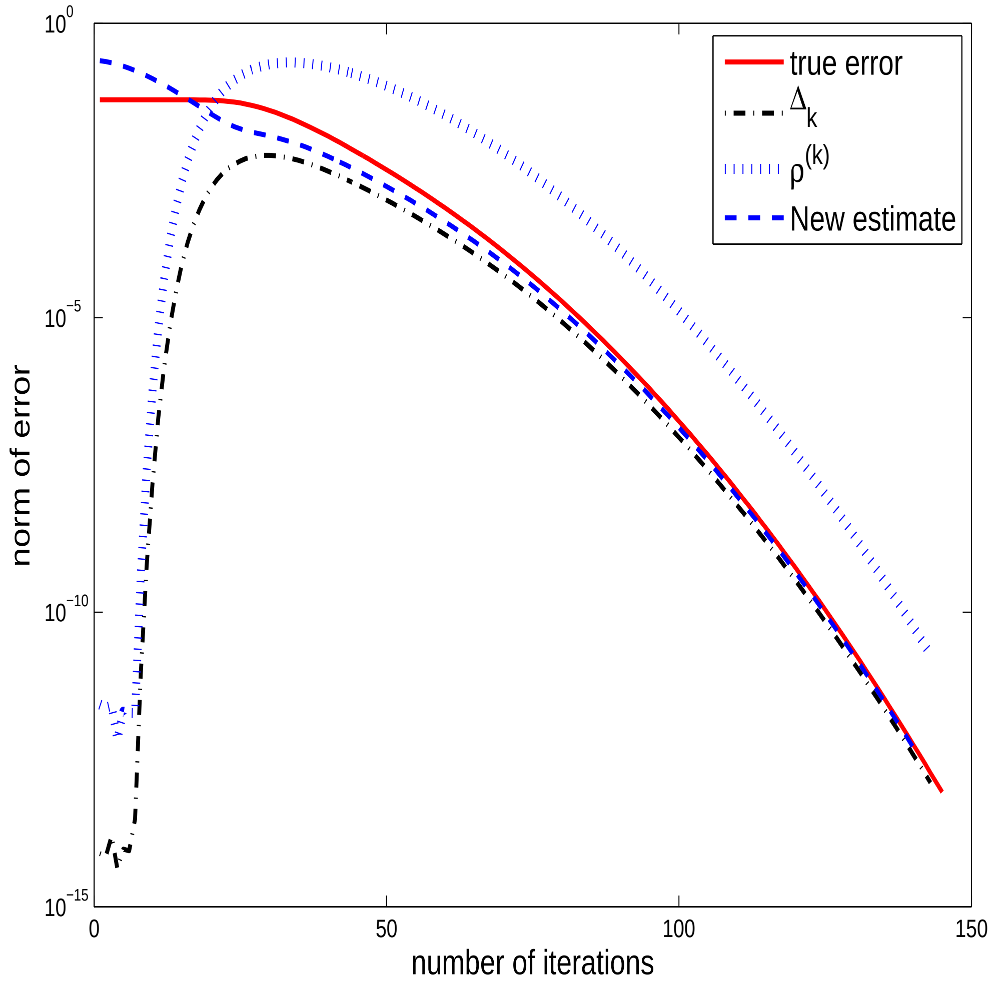
⋆ Computational cost only 3-5 additional iterations

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



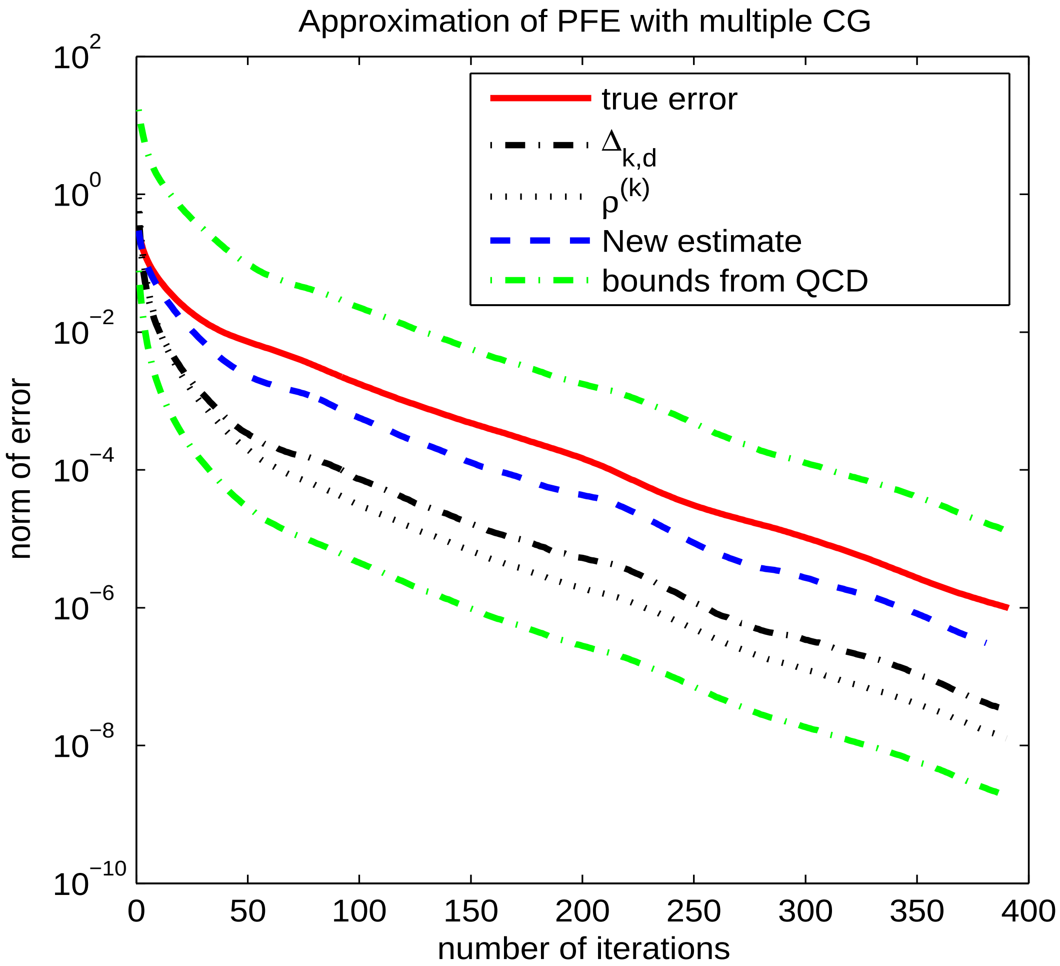
Note: superlinear convergence

“complex” CG for A sym-spd and $f(\lambda) = \exp(-\lambda)$: $\exp(-A)v$



Note: superlinear convergence

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



Approximation with Krylov subspaces

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

V_m s.t. range(V_m) $= \mathcal{K}_m(A, v)$ and $V_m^\top V_m = I$

$\Rightarrow$ Motivation: $\exists\, p$ polynomial (interpolatory): $f(A) = p(A)$

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"Classical" approach (e.g. Saad '92):

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

$$f(A)v \;\approx\; x_m = V_m f(H_m) e_1 \qquad \|v\| = 1$$

$\star$ x_m from interpolation pb. in Hermite sense: $V_m f(H_m) e_1 = p_{m-1}(A) v$

Krylov vs. Rational Approximation

$f \to \mathcal{R}_\nu$

Krylov: $\mathcal{R}_\nu(A)v \quad \approx \quad V_m \mathcal{R}_\nu(H_m)e_1$

$$\begin{aligned}
\mathcal{R}_\nu(A)v &= \omega_0 v + \sum_{j=1}^{\nu} \omega_j (A - \xi_j I)^{-1} v \\
&\approx \omega_0 v + \sum_{j=1}^{\nu} \omega_j V_m (H_m - \xi_j I)^{-1} e_1 \\
&= V_m \left(\omega_0 e_1 + \sum_{j=1}^{\nu} \omega_j (H_m - \xi_j I)^{-1} e_1 \right) \equiv V_m \mathcal{R}_\nu(H_m) e_1
\end{aligned}$$

$V_m \mathcal{R}_\nu(H_m)e_1$ term-by-term Galerkin projection

(van der Vorst, '87, Lopez & S., '06)

Approximation of $\exp(-A)v$ in $\mathcal{K}_m$. I

Typical convergence estimates (Hochbruck & Lubich '97)

A sym. semidef.

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

$$\|\exp(-A)v - V_m \exp(-H_m)e_1\| \leq \frac{10}{\rho} e^{-\rho} \left(\frac{e\rho}{m}\right)^m, \quad m \geq 2\rho$$

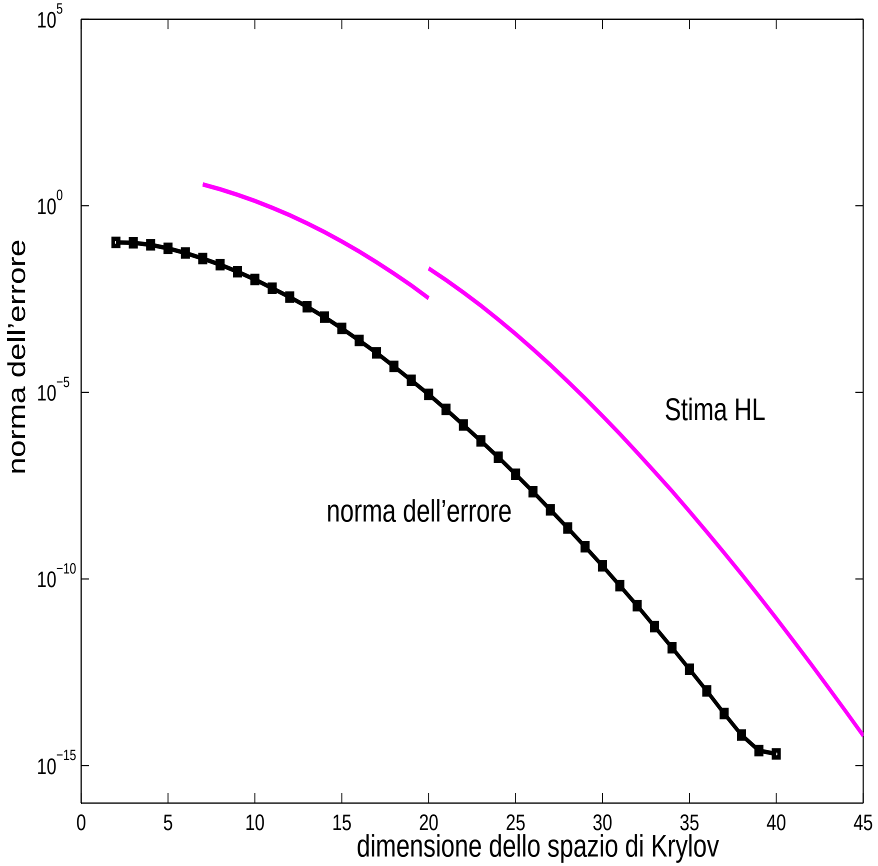
where $\sigma(A) \subseteq [0, 4\rho]$

see also Tal-Ezer '89, Druskin & Knizhnerman '89, Stewart & Leyk '96

Other similar estimates for $\lambda^{-1/2}, \cosh, ecc.$

Typical plot for the error

$$\| \exp(-A)v - V_m \exp(-H_m)e_1 \|$$



Superlinear convergence

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

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

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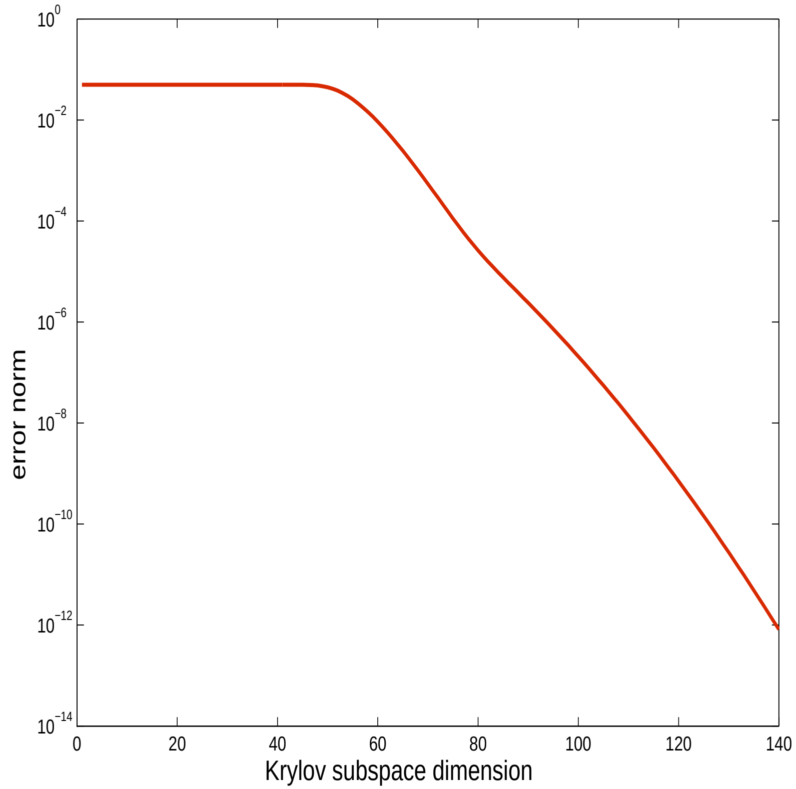
	Euler		Exp	
step δt	CPU	error	CPU	error (#its*)
0.001	1.9	$2 \cdot 10^{-3}$	0.09	$9 \cdot 10^{-4}$(37)
0.005	0.4	$1 \cdot 10^{-2}$	0.07	$4 \cdot 10^{-3}$(28)
0.01	0.2	$2 \cdot 10^{-2}$	0.05	$1 \cdot 10^{-2}$(25)

* : Stopping criterion tolerance related to timestep

$\Rightarrow$ More general exponential integrators

...When things are not so easy

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



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

Acceleration Techniques

$\star$: Improving approximation space

- Spectral approximation : $\mathcal{K}_m((I+\gamma A)^{-1}, v)$, $\gamma > 0$

$$f(A)v \quad \approx \quad V_m f(\frac{1}{\gamma}(H_m^{-1} - I))e_1$$

(Moret & Novati '04, van den Eshof & Hochbruck, '06, Popolizio & S. '08)

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- "Extended" space: $\mathcal{K}_m(A^{-1}, v) \cup \mathcal{K}_m(A, v)$

$$f(A)v \quad \approx \quad \mathcal{V}_m f(\mathcal{T}_m)e_1, \qquad \mathcal{T}_m = \mathcal{V}_m^\top A \mathcal{V}_m$$

(Druskin & Knizhnerman,'98, Simoncini,'07)

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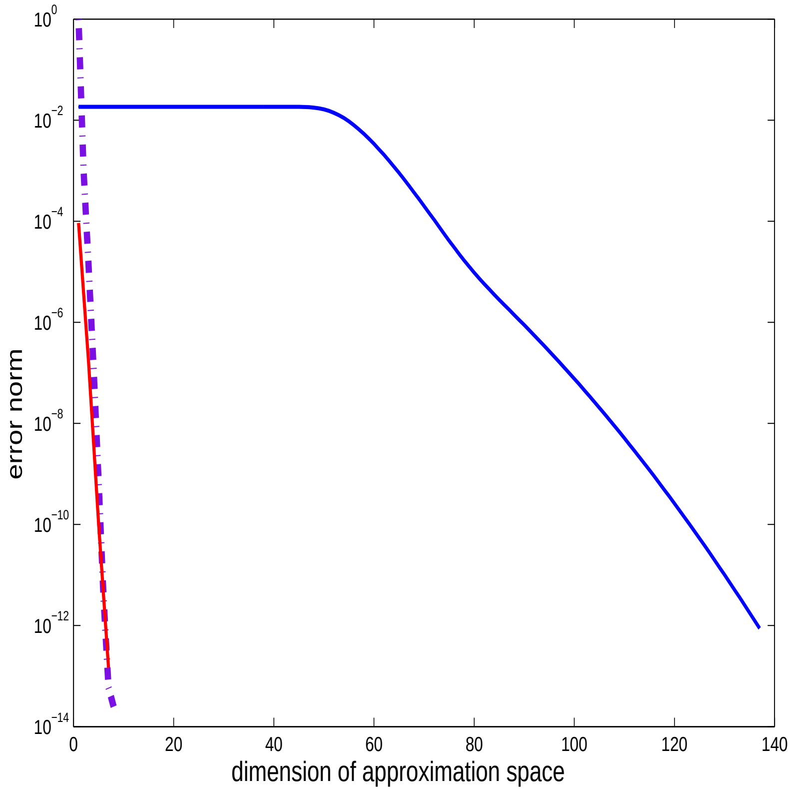
(Druskin & Knizhnerman,'98, Simoncini,'07)

$\star$: Relaxing optimality properties

- *Local* orthogonality of the basis (Eiermann & Ernst '06)
- Limit costs of rational approx. with $\mathcal{R}_\nu(A)v$ (Popolizio & S. '08)

Acceleration

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



-: std Krylov   -.: Spectral accel.   -: "extended" space

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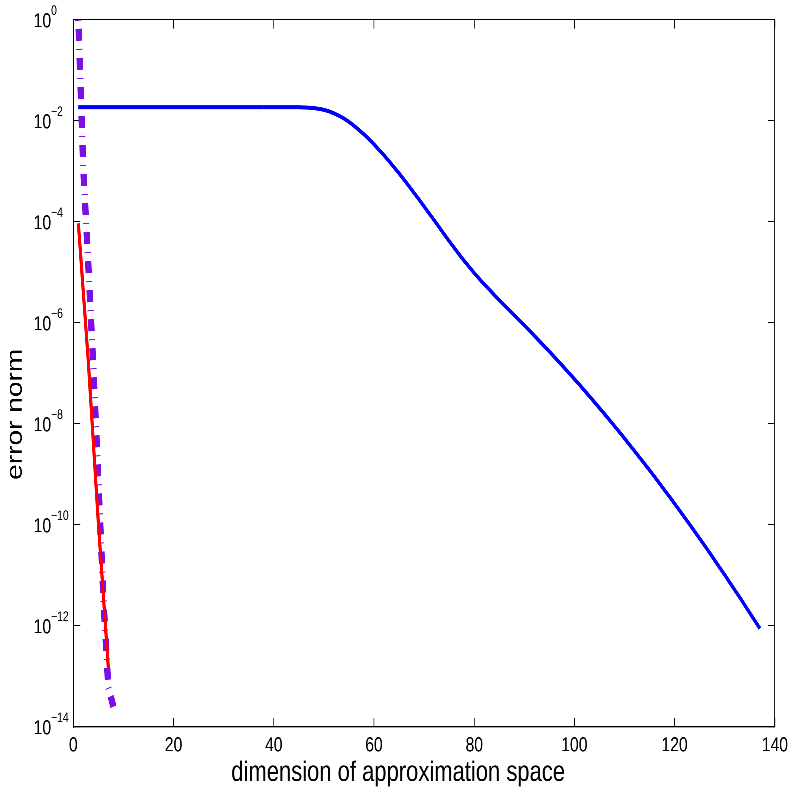
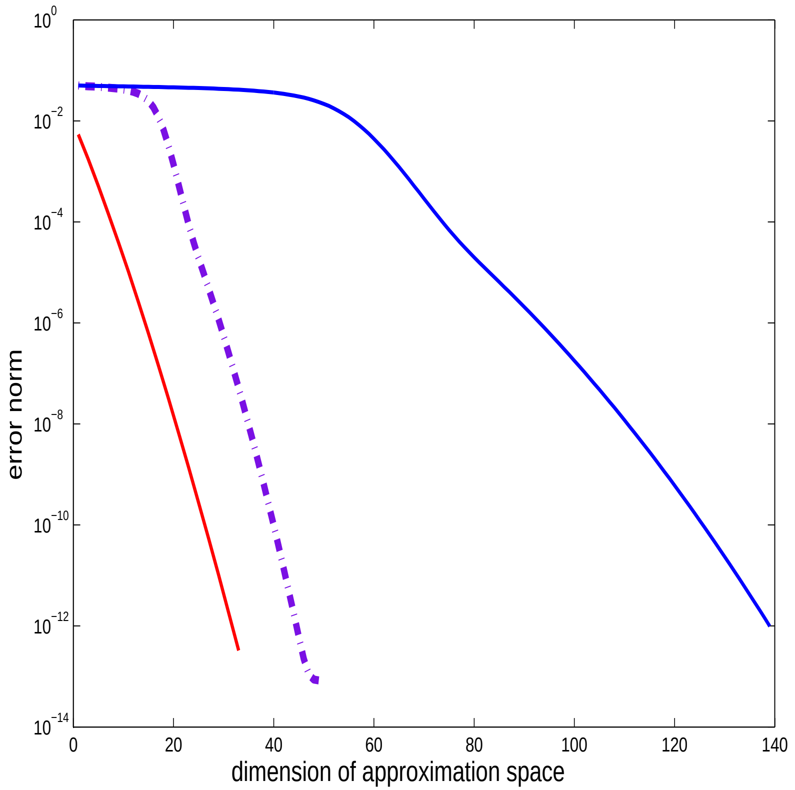


$f(\lambda) = \lambda^{-1/2}$



-: std Krylov -.: Spectral accel. -: "extended" space

Applications. II

Lyapunov Equation:

$$AX + XA^\top + Q = 0$$

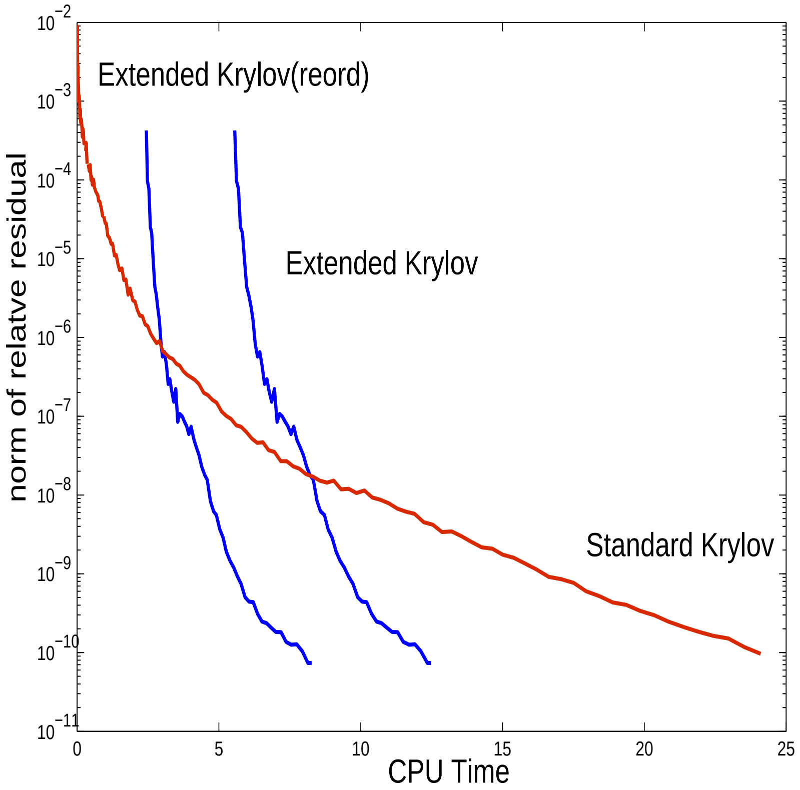
with $-A$ dissipative, $Q = BB^\top$ low rank

$$X = \int_0^\infty e^{-tA} BB^\top e^{-tA^\top} dt = \int_0^\infty x x^\top dt$$

with $x = \exp(-tA)B$

An example. “Time-invariant” linear systems

$$\mathbf{x}' = \mathbf{x}_{xx} + \mathbf{x}_{yy} + \mathbf{x}_{zz} - 10x\mathbf{x}_x - 1000y\mathbf{x}_y - 10\mathbf{x}_z + \mathbf{b}(x,y)\mathbf{u}(t)$$



space dim. : 146 (Standard Krylov) 112 (“extended” Krylov) $A \in \mathbb{R}^{18^3 \times 18^3}$

Simoncini,’07

Applications. Ill-posed problem. I

$$
\begin{cases}
u_{zz} - Lu = 0, \qquad (x, y, z) \in \Omega \times [0, z_1] \\
u(x, y, z) = 0, \qquad (x, y, z) \in \partial\Omega \times [0, z_1] \\
u(x, y, 0) = g(x, y), \qquad (x, y) \in \Omega \\
u_z(x, y, 0) = 0, \qquad (x, y) \in \Omega
\end{cases}
$$

L elliptic oper., linear, self-adjoint, positive def.

Pb: determine u for $z = z_1$: $\quad f(x, y) = u(x, y, z_1),\ (x, y) \in \Omega$.

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Pb: determine u for $z = z_1$: $f(x,y) = u(x,y,z_1)$, $(x,y) \in \Omega$.

Separation of variables: $u(x,y,z) = \cosh(z\sqrt{L})g$

$\star$: L unbounded $\Rightarrow$ $\cosh(z\sqrt{L})g$ unstable (wrto data perturbations)

L. Eldén & S., in prep.

Applications. Ill-posed problem. II

Regularization: $\widetilde{g}$ perturbed data

$$u(x,y,z) = \sum_{k=1}^{\infty} \cosh(\lambda_k z)\, \langle s_k, g\rangle\, s_k(x,y)$$

$$\Rightarrow\ v(x,y,z) = \sum_{\lambda_k \le \lambda_c} \cosh(\lambda_k z)\, \langle s_k, \widetilde{g}\rangle\, s_k(x,y)$$

(λ_k^2, s_k) eigenpairs of L

Applications. Ill-posed problem. II

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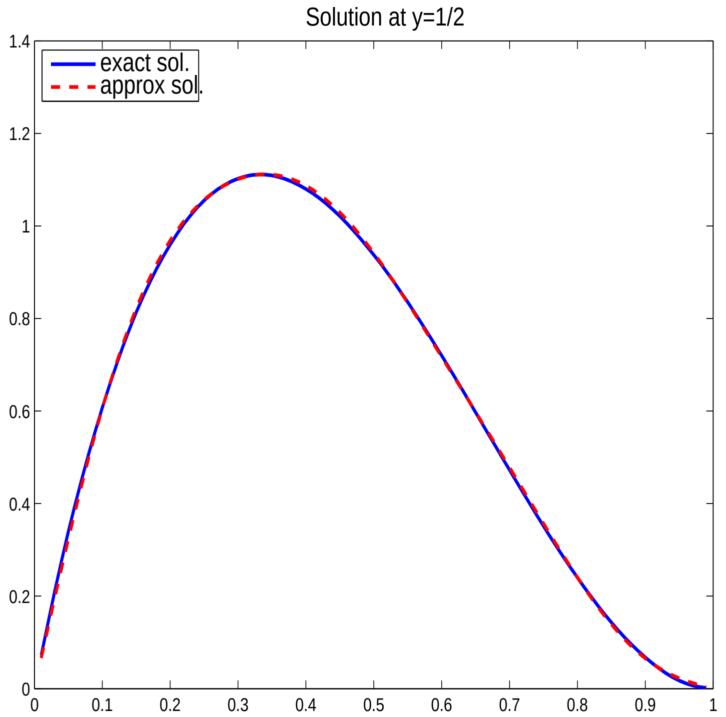
Approx, for instance, in Krylov subspace $\mathcal{K}_m(L, \widetilde{g})$:

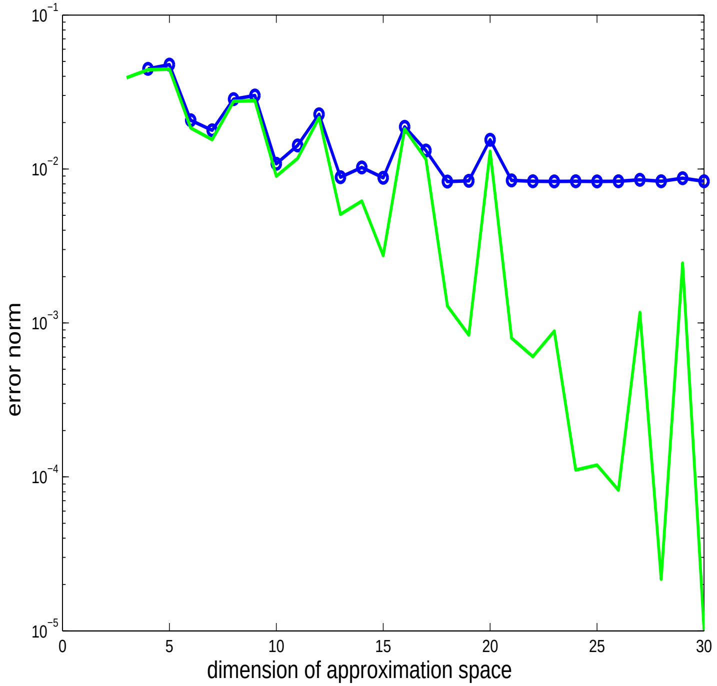
$$u^{(m)}(z) = V_m \cosh(z\sqrt{H_m}) e_1 \|g\| \quad \Rightarrow$$

$$\Rightarrow v^{(m)}(z) = V_m \sum_{\theta_j^{(m)} \le \lambda_c} y_j^{(m)} \cosh(z\theta_j^{(m)}) (y_j^{(m)})^\top e_1 \| \quad \|$$

$((\theta_j^{(m)})^2, y_j^{(m)})$ eigenpairs of H_m

Applications. Ill-posed problem. III





Functional error: - $\|v(z) - v^{(m)}(z)\| \quad z = 0.1$

Perturbation error : - $\|u(z) - v^{(m)}(z)\| \quad z = 0.1$

Conclusions

- Great potential of using $f(A)v$ in application problems
- Exploit low cost of using A instead of $f(A)$
- Further developments in acceleration techniques
- The case of A nonsymmetric

Related References

- L. Lopez and V. S., *Analysis of projection methods for rational function approximation to the matrix exponential* SIAM J. Numerical Analysis, v. 44, n. 2 (2006), pp. 613 - 635.
- L. Lopez and V. S., *Preserving geometric properties of the exponential matrix by block Krylov subspace methods* BIT, Numerical Mathematics, v. 46, n.4 (2006), pp. 813-830.
- V. S., *A new iterative method for solving large-scale Lyapunov matrix equations* SIAM J. Scient. Computing, v.29, n.3 (2007), pp. 1268-1288.
- A. Frommer and V. S., *Stopping criteria for rational matrix functions of Hermitian and symmetric matrices* March 2007. To appear in SIAM J. Scientific Computing.
- M. Popolizio and V. S., *Acceleration Techniques for Approximating the Matrix Exponential Operator* October 2006. To appear in SIAM J. Matrix Anal. Appl.
- A. Frommer and V. S., *Matrix functions* March 2006.To appear in "Model Order Reduction: Theory, Research Aspects and Applications", Schilders, Wil H. A. and van der Vorst, Henk A. eds, Springer, Heidelberg.