# The Extended Krylov Subspace for Matrix Function Approximations: Analysis and Applications

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## The Problem

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

$$x = f(A)v$$

$\star$ $A$ large dimensions, $\|v\| = 1$

Applications:

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

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## Projection-type methods

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

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

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

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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 $\gamma$
- Rational Krylov subspace, for some $\omega_1, \omega_2, \ldots$
  $\mathcal{K} = \mathrm{span}\{v, (A - \omega_1 I)^{-1} v, (A - \omega_2 I)^{-1} v, \ldots\}$
- 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.

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 $V_m^\top V_m = I_m$:

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

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 (Saad '92)

## Acceleration Procedures: Shift-Invert Krylov

Choose $\gamma$ 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 $\gamma$: $A$ spd, $\gamma = \frac{1}{\sqrt{\lambda_{\min}\lambda_{\max}}}$ (Moret, 2009)

$A$ nonsym, (Beckermann-Reichel tr2008)

## Acceleration Procedures: Restarted Krylov

$$AV_m^{(1)} = V_m^{(1)} H_m^{(1)} + v_{m+1}^{(1)} h_{m+1,m}^{(1)} e_m^\top \quad (V_m^{(1)})^\top V_m^{(1)} = I$$
$$AV_m^{(2)} = V_m^{(2)} H_m^{(2)} + v_{m+1}^{(2)} h_{m+1,m}^{(2)} e_m^\top \quad (V_m^{(2)})^\top V_m^{(2)} = I$$

with $V_m^{(2)} e_1 = v_{m+1}^{(1)}$. Then

$$A[V_m^{(1)}, V_m^{(2)}] = [V_m^{(1)}, V_m^{(2)}] \widehat{H}_{2m} + v_{m+1}^{(2)} h_{m+1,m}^{(2)} e_{2m}^\top,$$

with

$$\widehat{H}_{2m} = \begin{bmatrix} H_m^{(1)} & 0 \\ e_1 h_{m+1,m}^{(1)} e_m^\top & H_m^{(2)} \end{bmatrix}.$$

Therefore (Eiermann-Ernst, '06)

$$\begin{aligned} f(A)v &\approx x_m^{(1)} = V_m^{(1)} f(H_m^{(1)}) \\ &\approx x_m^{(2)} = V_m^{(1)} f(H_m^{(1)}) e_1 + V_m^{(2)} f(\widehat{H}_{2m}) e_1|_{(2)} \\ & \qquad x_m^{(2)} = x_m^{(1)} + V_m^{(2)} f(\widehat{H}_{2m}) e_1|_{(2)} \end{aligned}$$

## Acceleration Procedures: Extended Krylov

For $A$ nonsingular,

$\mathcal{K} = K_{m_1}(A, v) + K_{m_2}(A^{-1}, A^{-1}v),$ Druskin-Knizhnerman 1998, $A$ 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

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

⋆ *Block* Arnoldi-type recurrence:

- $U_1 \leftarrow \mathrm{orth}([v, A^{-1}v])$

- $U_{j+1} \leftarrow [AU_j(:,1), A^{-1}U_j(:,2)] +$ 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, 2007

## 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 $d\mu(\zeta)$)

Druskin-Knizhnerman 1998:

$A$ sym: $\quad \|x - x_m\| = \mathcal{O}\left( m^2 e^{-2m \sqrt[4]{\frac{\lambda_{\min}}{\lambda_{\max}}}} \right)$

## Extended Krylov: Convergence theory II

For nonsingular $A$, with $0 \notin W(A)$, let $f = f_1 + f_2$, $a \in [0, \infty)$. Then

$$\|f_1(z) - \sum_{k=0}^{m-1} \gamma_{1,k} F_{1,k}(z)\| \le \frac{c_1}{\Phi_1(-a)^m},$$

$$\|f_2(z) - \sum_{k=0}^{m-1} \gamma_{2,k} F_{2,k}(z^{-1})\| \le \frac{c_2}{\Phi_2(-\frac{1}{a})^m},$$

$\Phi_j$, $F_{j,k}$, $j = 1, 2$ conformal map and Faber Polyn 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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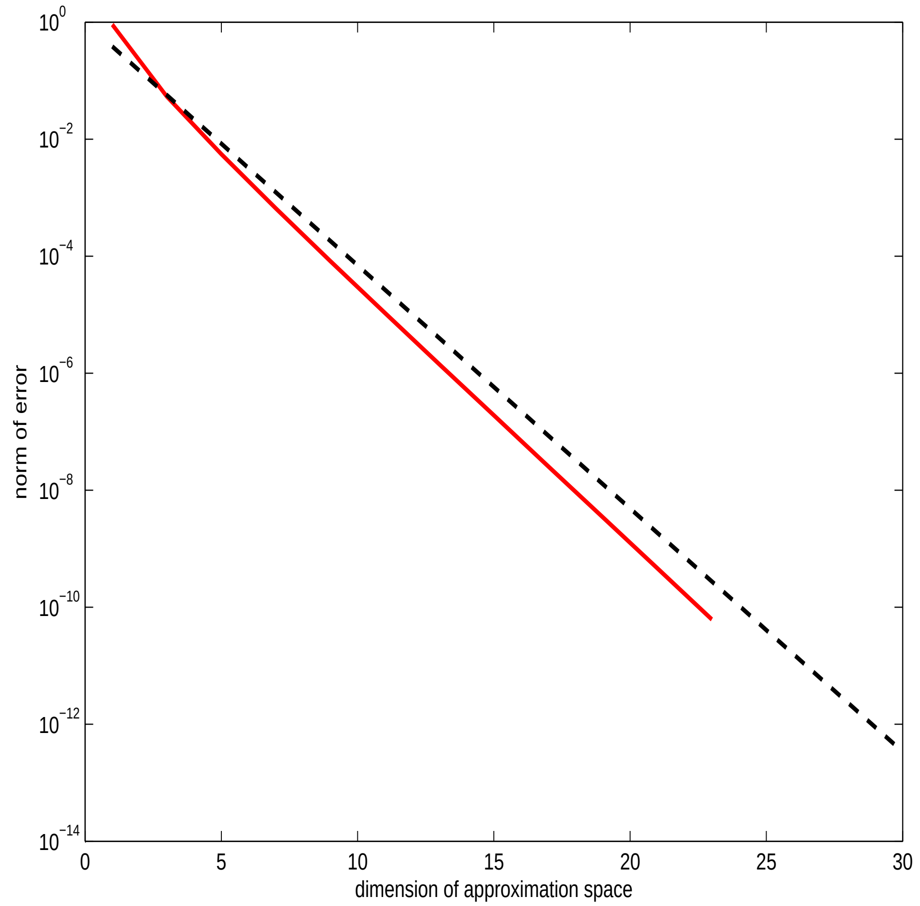
e.g. for $A$ symmetric ($\Phi_1, \Phi_2$ known, $a = \sqrt{\lambda_{\min}\lambda_{\max}}$) :

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

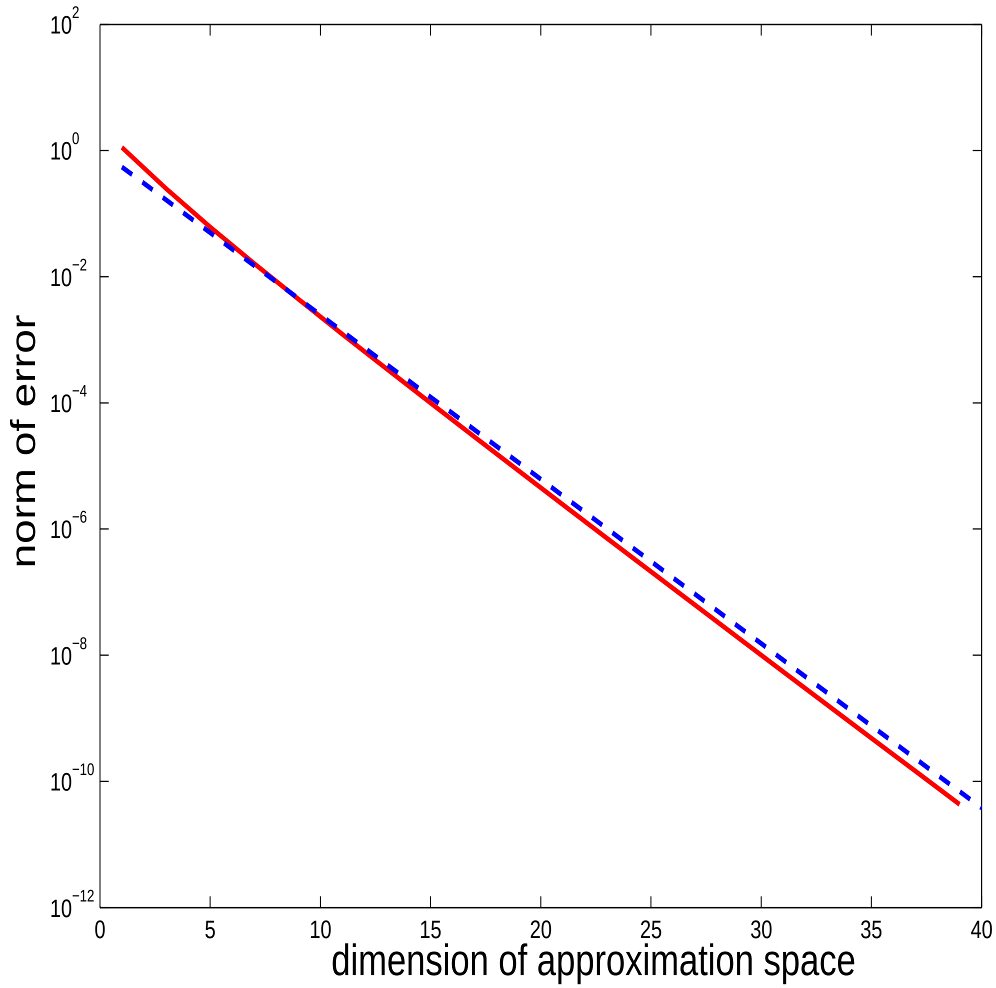
## Convergence rate. $A \in \mathbb{R}^{400\times 400}$ spd. $f(\lambda) = \lambda^{-1/2}$




$\sigma(A) \subseteq [1, 50]$

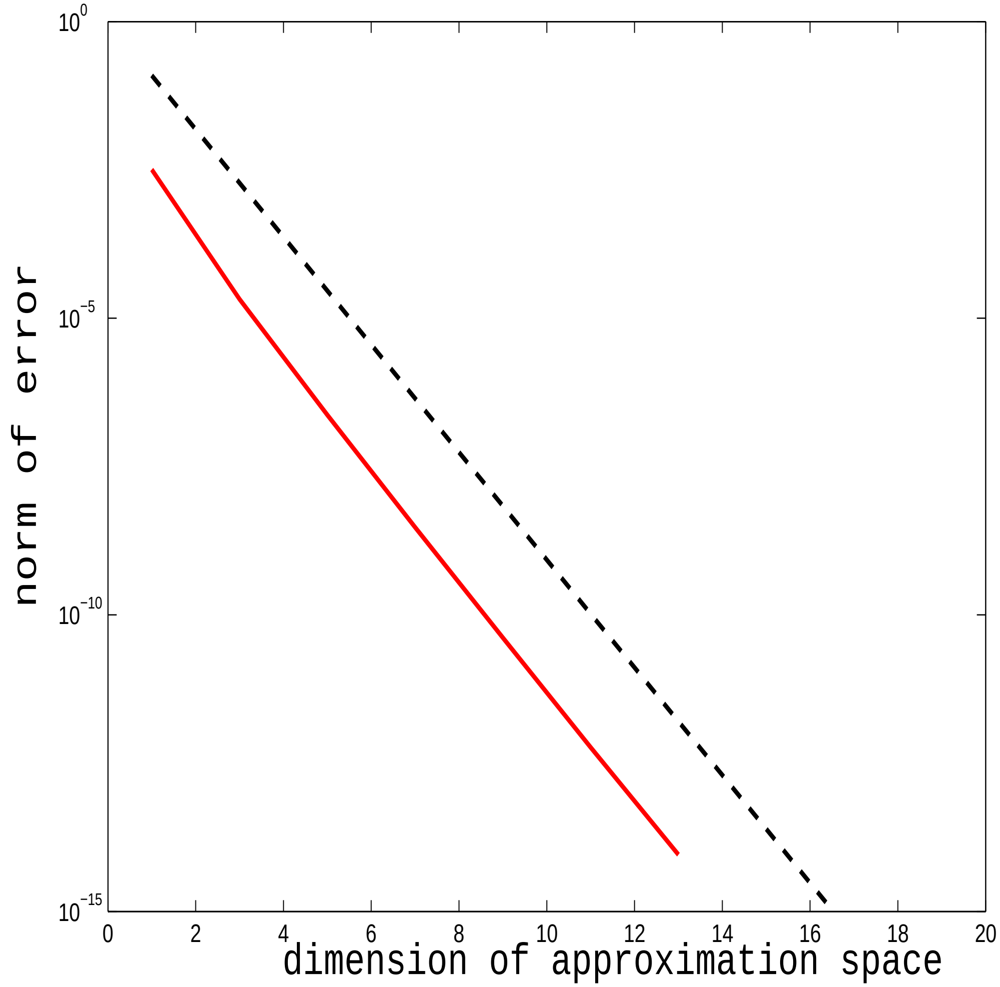
Uniform spectral distribution

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




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

## Experiment. $A \in \mathbb{R}^{200\times 200}$ Jordan block, $\lambda = 4$. $f(\lambda) = \lambda^{1/2}$




$W(A)$ disk centered at $\lambda$ and unit radius

## Large-scale numerical experiments

$A$ from FD discretization of

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

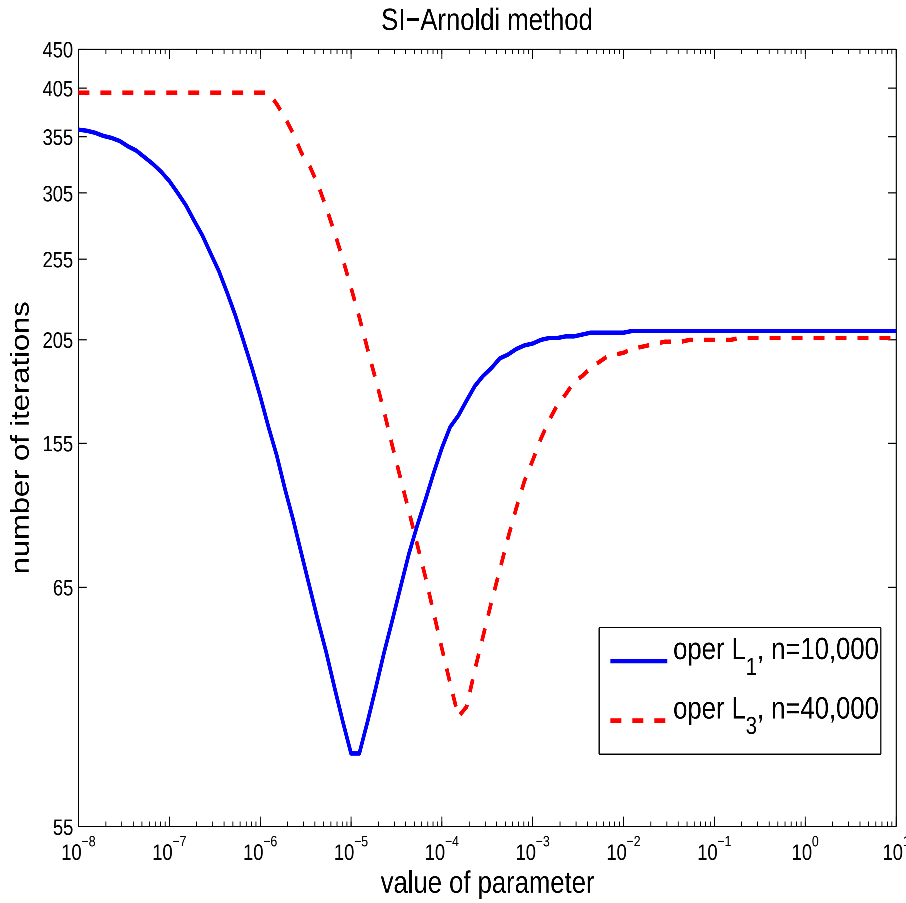
on unit square/cube, Dirichlet hom. bc.

### Inner system solves:

- Extended Krylov: systems with $A$ solved with GMRES/AMG
- SI-Arnoldi: systems with $I + \gamma A$ solved with IDR($s$)/ILU

# An intermezzo

SI-Arnoldi requires getting the parameter $\gamma$:




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

## Comparisons: CPU Time in Matlab (space dim.)

| $f$ | Oper. | $n$ | SI-Arnoldi | EKSM | Std Krylov |
|---|---|---|---|---|---|
| $\lambda^{1/2}$ | $\mathcal{L}_1$ | 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 |
|---|---|---|---|---|---|
| $\lambda^{-1/3}$ | $\mathcal{L}_1$ | 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:

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

## 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) |

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

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

A special case: $f(\lambda) = (\lambda - \sigma)^{-1}$. $x = (A - \sigma I)^{-1} v \equiv f_\sigma(A) v$

All as before - and new perspective:

- Many shifts in a wide range (e.g., Structural dynamics, electromagn.)

$$(A - \sigma_j I)x = v, \qquad \sigma_j \in [\alpha, \beta], \quad \text{large interval}$$

$j = 1, \ldots, k, \;\; k = \mathcal{O}(100)$

- Few shifts (e.g., quadrature formulas)

$$z = \sum_{j=1}^{k} \omega_j (A - \sigma_j I)^{-1} v$$

- Transfer function

$$h(\sigma) = c^*(A - i\sigma I)^{-1} b, \quad \sigma \in [\alpha, \beta]$$

## Shifted systems

Extended Krylov subspace method:

$$x \approx \mathcal{U}_m f_\sigma(\mathcal{T}_m) e_1 = \mathcal{U}_m (\mathcal{T}_m - \sigma I)^{-1} e_1$$

standard Galerkin-type approximation for shifted systems

(cf. FOM, CG, ...)

Key fact: A single $\mathcal{K}$ for all shifted systems.

Shift invariance:

$$K_m(A, v) = K_m(A + \sigma I, v)$$

Note: Solve systems with $A$ to approximate $(A + \sigma I)^{-1} v$

## Added feature: restarting made easy

$$A\mathcal{U}_m = \mathcal{U}_m \mathcal{T}_m + U_{m+1} \boldsymbol{\tau} E_m^\top$$

Proportionality of the residuals:

For $x_m(\sigma) = \mathcal{U}_m(\mathcal{T}_m - \sigma I)^{-1} e_1$, the residual

$$r_m(\sigma) := b - (A - \sigma I) x_m(\sigma), \qquad r_m(\sigma) \propto \mathcal{U}_{m+1} e_{2m+1} \quad \forall \sigma$$

(typical of Galerkin-type procedures)

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**Restarting with a single approximation space:**

$$\mathcal{K}^{(2)} = K_m(A, v^{(2)}) + K_m(A^{-1}, A^{-1} v^{(2)}), \qquad v^{(2)} = \mathcal{U}_{m+1} e_{2m+1}$$

$$x_m^{(2)}(\sigma) = x_m^{(1)}(\sigma) + z_m, \qquad z_m \in \mathcal{K}^{(2)}$$

## An example from Structural Dynamics

$$(K^\star - \sigma^2 M)x = b, \qquad \Rightarrow \; (K^\star M^{-1} - \sigma^2 I)\hat{x} = b$$

$K^\star$ stiffness + hysteretic damping, $M$ mass $\sigma \in 2\pi[0.1, 60.1]$ frequencies, $n = 3627$

number of restarts (subspace dimension)

| restarted EKSM | restarted FOM |
|---|---|
| 3 (20) | - (20) |
| 1 (34) | 81(40) |
| | 21(80) |

## Transfer function approximation (cf. MOR)

$$h(\sigma) = c^*(A - i\sigma I)^{-1}b, \quad \sigma \in [\alpha, \beta]$$

Given space $\mathcal{K}$ and $V$ s.t. $\mathcal{K}$=range$(V)$,

$$h(\sigma) \approx (V^*c)^*(V^*AV - \sigma I)^{-1}(V^*b)$$

For $\mathcal{K} = K_m(A, b)$ (standard Krylov):

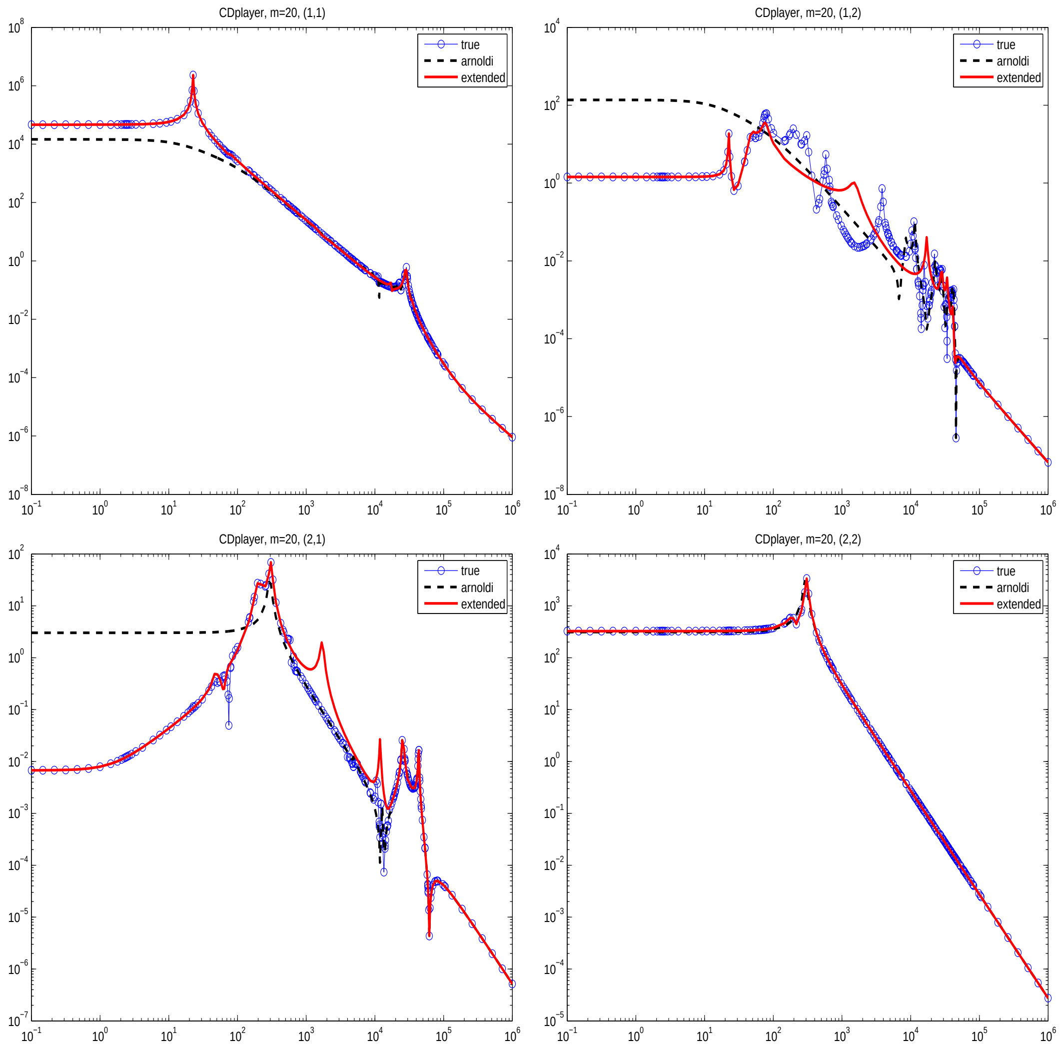
$$h_m(\sigma) = (V_m^*c)^*(H_m - \sigma I)^{-1}e_1\|b\|$$

For $\mathcal{K} = K_m(A, b) + K_m(A^{-1}, A^{-1}b)$ (EKSM):

$$h_m(\sigma) = (\mathcal{U}_m^*c)^*(\mathcal{T}_m - \sigma I)^{-1}e_1\|b\|$$

Alternative: Rational Krylov (Grimme-Gallivan-VanDooren etc. )
choosing the poles unresolved issue

# An example: CD Player, $|h(\sigma)| = |C^*_{:,i}(A - i\sigma I)^{-1}B_{:,j}|$



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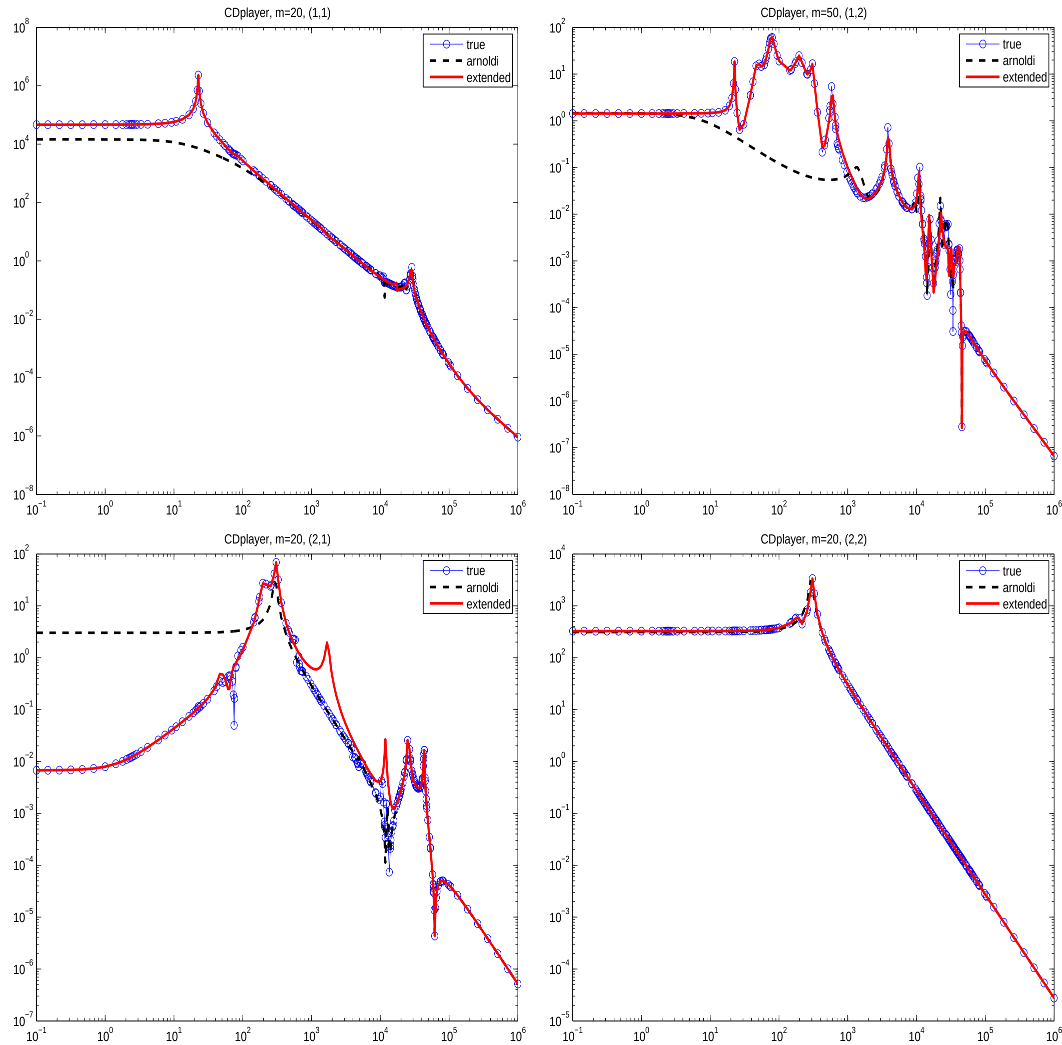

## Two-parameter linear systems

$$(A + \beta_j B + \alpha_i I)x = v, \qquad x = x(\alpha_i, \beta_j)$$

Commonly: $\#\alpha = O(100), \quad \#\beta = O(10)$

Problem: Solve all systems at a cost sublinear in $\#\alpha, \#\beta$

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Commonly: $\#\alpha = O(100), \quad \#\beta = O(10)$

Problem: Solve all systems at a cost sublinear in $\#\alpha, \#\beta$

Currently, Shifted restarted EKSM most efficient strategy:

For each $\beta_j$, solve $(A+\beta_j B+\alpha_i I)x = v, \quad \forall \alpha_i$

But: linear in $\beta$...

## Conclusions

- Efficient generation of the Extended Krylov subspace
- Complete theory for EKSM for a large class of functions
- Performance:

  - Competitive with respect to available methods

  (when solving with $A$ can be made cheap)

  - Does not depend on parameters

  - Projection-type method: wide applicability (work in progress)

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