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

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Partially joint work with Leonid Knizhnerman, Moscow

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. $\exp(\lambda), \sqrt{\lambda^{-1}}, \cos(\lambda), \ldots$)
- Inverse Problems $(\exp(\lambda), \cosh(\lambda), \ldots)$
- 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 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.

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:

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

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 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, 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)

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

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

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

⋆ *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, 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 $d\mu(\zeta)$)

Extended Krylov: Convergence theory II

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

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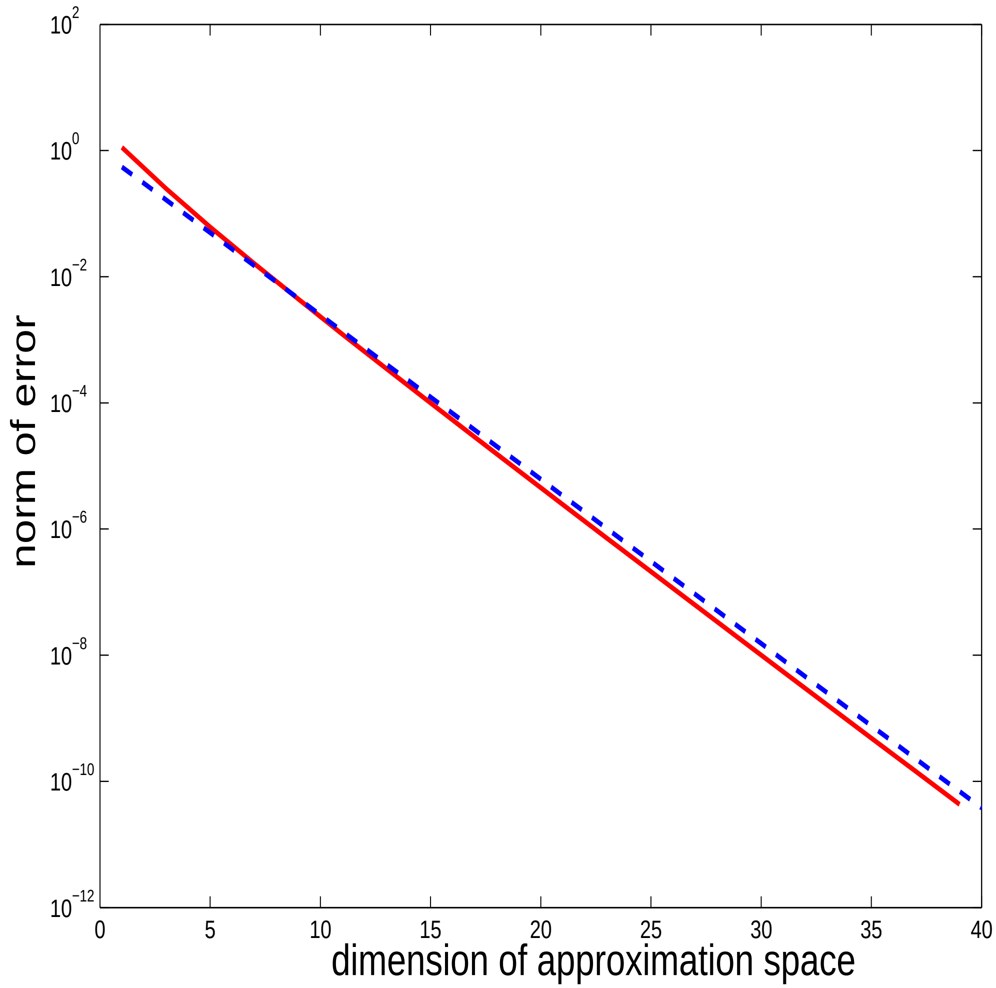
e.g. for A symmetric (Φ_1, Φ_2 known, $a = \sqrt{\lambda_{\min}\lambda_{\max}}$) :

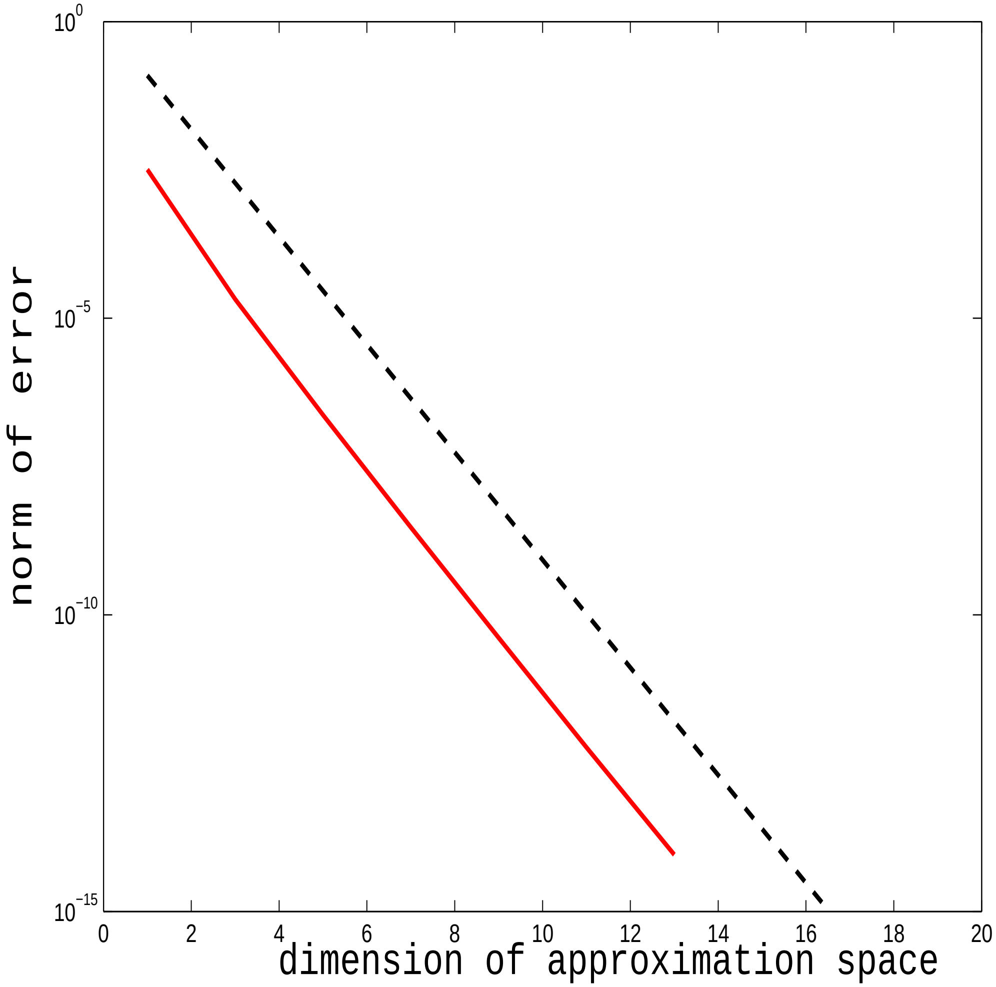
$\|x - x_m\| = O(\exp(-2m \sqrt[4]{\frac{\lambda_{\min}}{\lambda_{\max}}}))$

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



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

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



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

Large-scale numerical experiments

A from FD discretization of

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

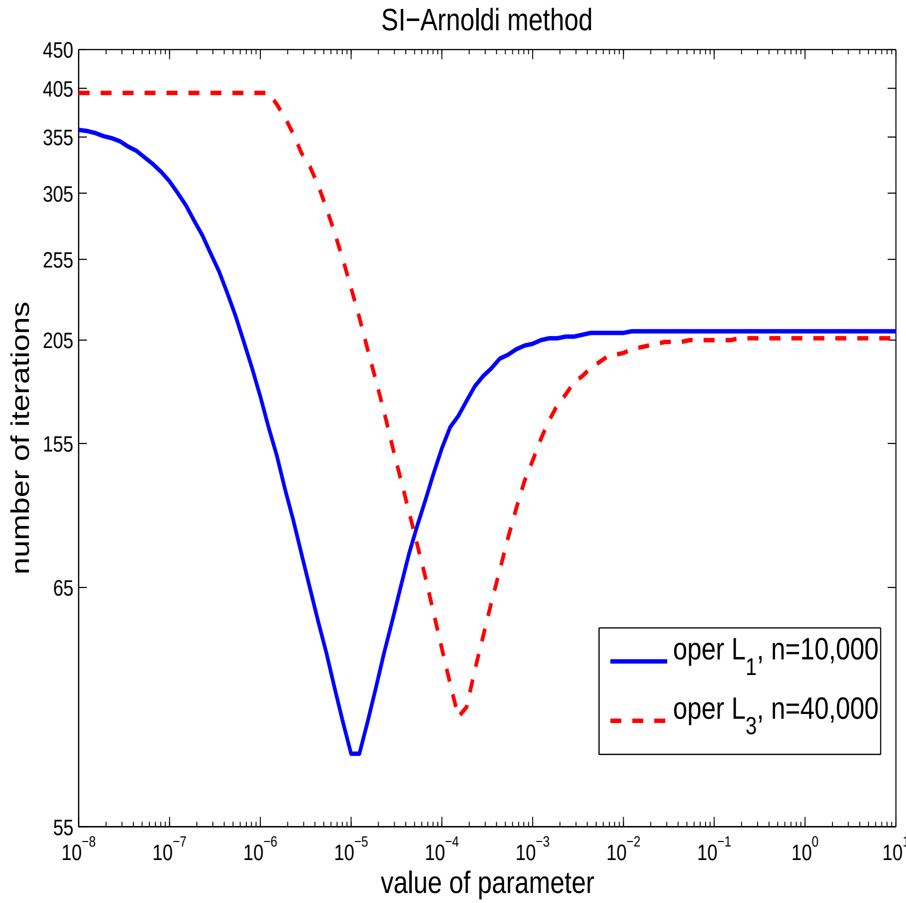
on unit square/cube, Dirichlet hom. bc.

Inner system solves:

- Extended Krylov: systems with A solved with GMRES/AMG
- SI-Arnoldi: 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 $f(\lambda) = \lambda^{1/2}$

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:

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

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)

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

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

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 (joint work with A. Frommer)

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):

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

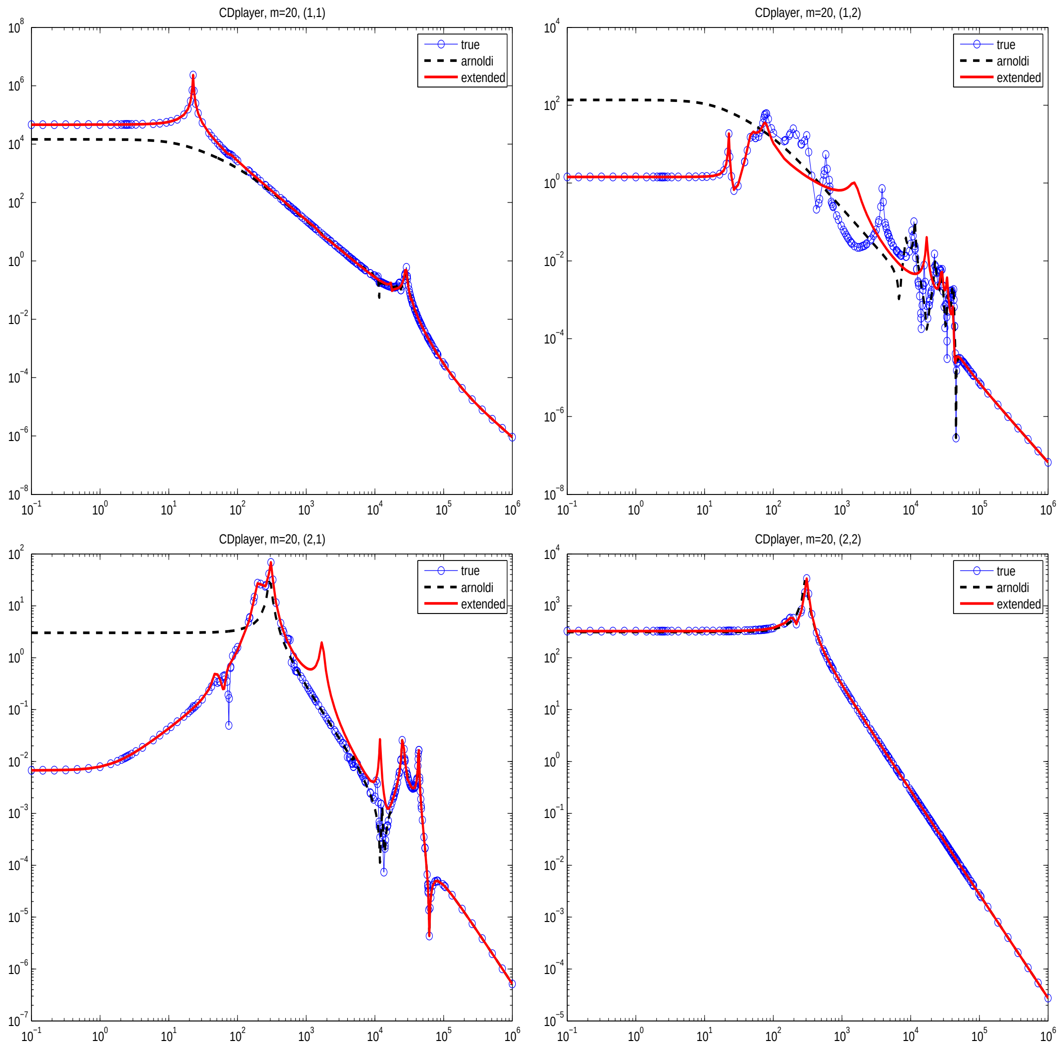
For $\mathcal{K} = K_m(A, b) + K_m(A^{-1}, A^{-1}b)$ (EKSM):

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

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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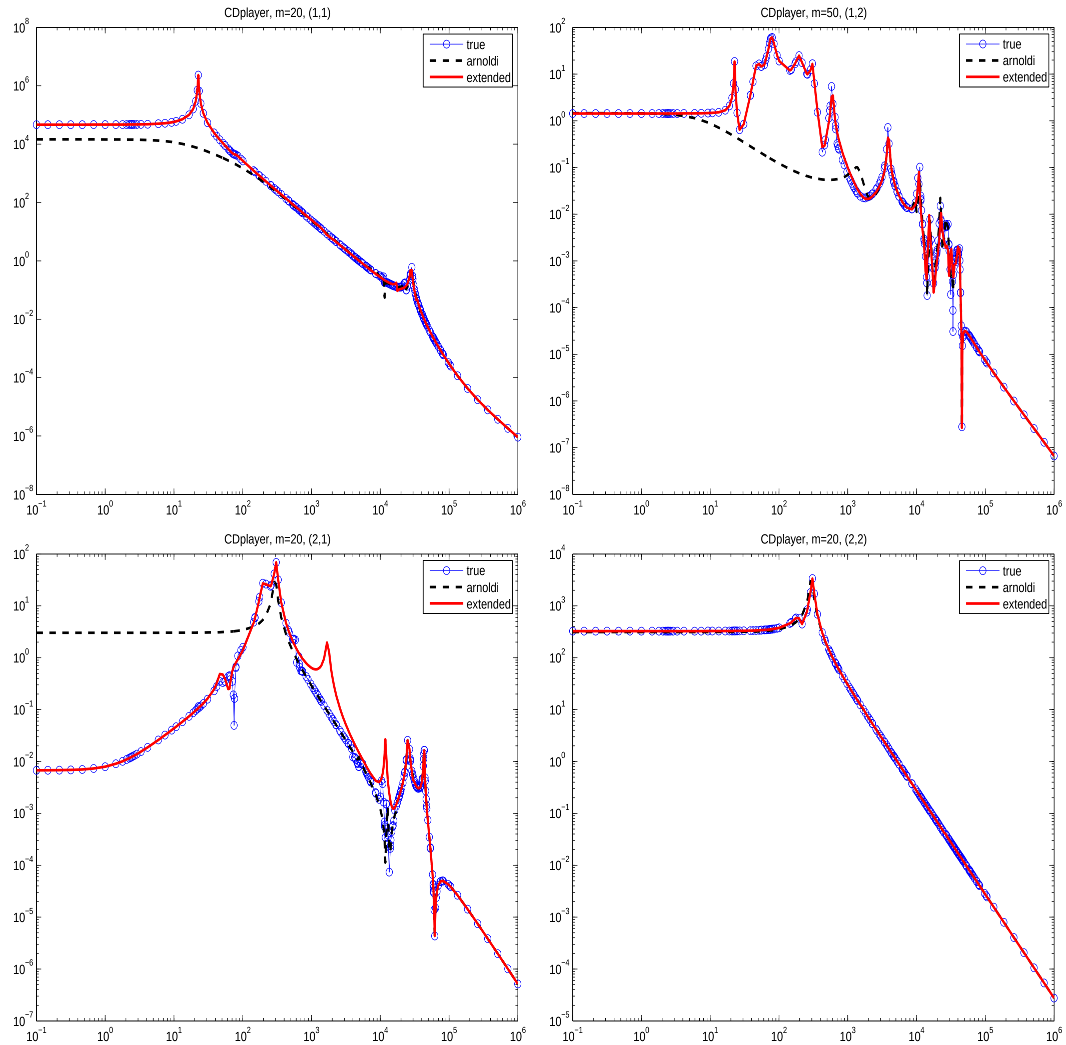

Two-parameter linear systems (with F. Perotti - K. Meerbergen)

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

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

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

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..The expensive way:

$$\left[\begin{pmatrix} A & & & \\ & A & & \\ & & \ddots & \\ & & & A \end{pmatrix} + \begin{pmatrix} \beta_1 B & & & \\ & \beta_2 B & & \\ & & \ddots & \\ & & & \beta_k B \end{pmatrix} + \alpha_i I \right] z = f$$

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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