Adaptive rational Krylov subspaces for large-scale dynamical systems

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joint work with Vladimir Druskin, Schlumberger Doll Research

Model Order Reduction

Given the continuous-time system

$$\mathbf{\Sigma} = \left(\begin{array}{c|c} A & B \\ \hline C & \end{array}\right), \quad A \in \mathbb{C}^{n \times n}$$

Analyse the construction of a reduced system

$$\hat{\mathbf{\Sigma}} = \left(\begin{array}{c|c} \tilde{A} & \tilde{B} \\ \hline \tilde{C} & \end{array}\right)$$

with $\tilde{A}$ of size $m \ll n$

Projection methods and Linear Dynamical Systems

Time-invariant linear system:

$$\mathbf{x}'(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{x}(0) = x_0$$
$$\mathbf{y}(t) = C\mathbf{x}(t)$$

- Approximation of the matrix Transfer function
- Solvers for the Lyapunov matrix equation

Emphasis: A large dimensions, $W(A) \subset \mathbb{C}^-$

Projection methods: the general idea

Given space $K \subset \mathbb{R}^n$ of size m and (orthonormal) basis V_m,

$$A \to A_m = V_m^* A V_m, \quad B \to B_m = V_m^* B, \quad C \to C_m = C V_m$$

Solve with A_m, B_m, C_m

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Choices of K in the literature:

- Standard Krylov subspace: $\quad K_m(A, B) = \mathrm{span}\{B, AB, \ldots, A^{m-1}B\}$

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- Shift-Invert Krylov subspace:
  $K_m((A - \sigma I)^{-1}, B) = \mathrm{span}\{B, (A - \sigma I)^{-1}B, \ldots, (A - \sigma I)^{-(m-1)}B\}$;
  often $\sigma = 0$

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  often $\sigma = 0$
- Extended Krylov subspace: $\mathbf{EK}_m(A, B) = K_m(A, B) + K_m(A^{-1}, A^{-1}B)$
- Rational Krylov subspace:
  $K_m(A, B, \mathbf{s}) = \mathrm{span}\{(A - s_1 I)^{-1}B, (A - s_2 I)^{-1}B, \ldots, (A - s_m I)^{-1}B\}$
  usually $\mathbf{s} = [s_1, \ldots, s_m]$ a-priori

Transfer function approximation

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

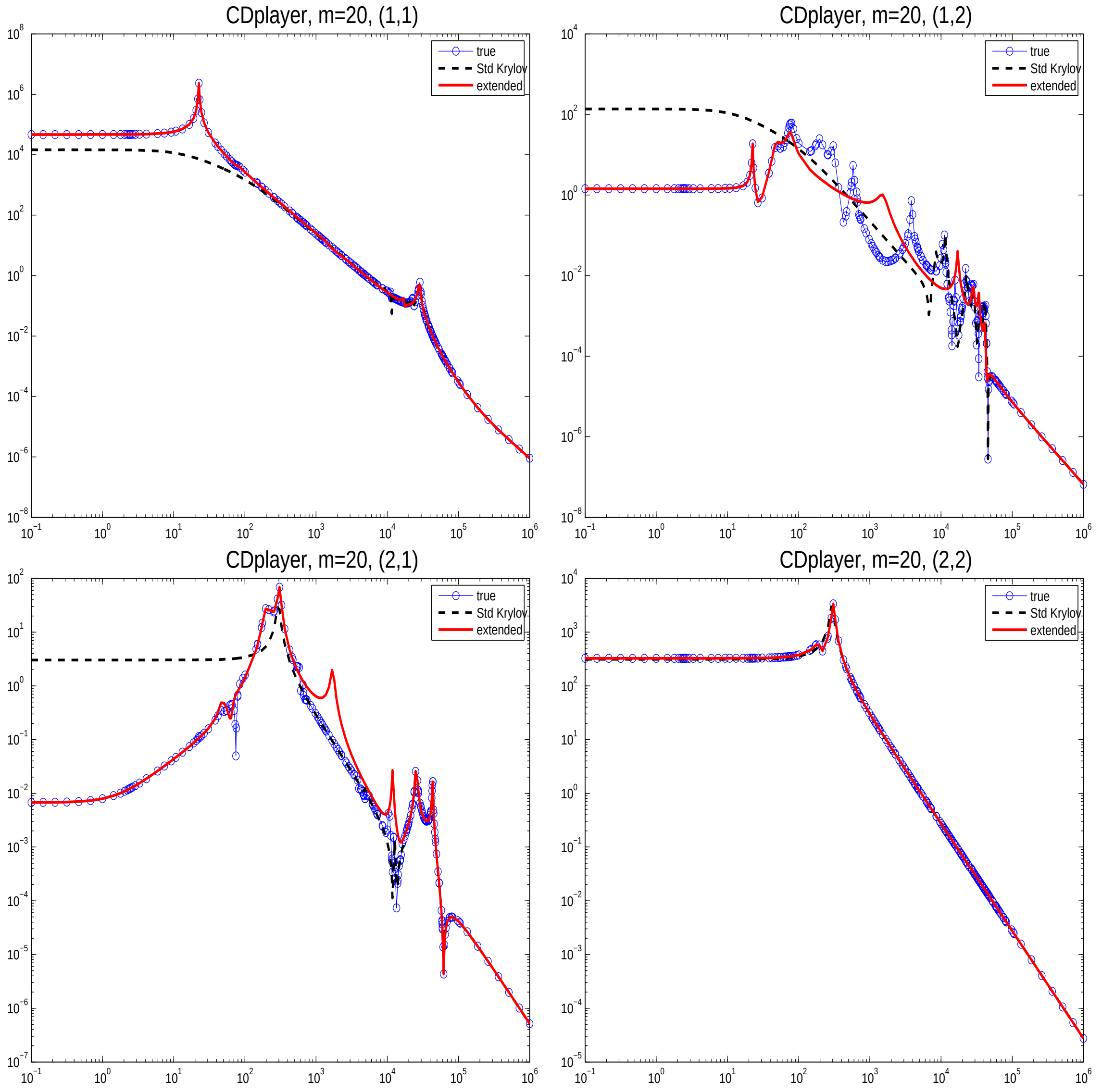
Given space $\mathcal{K}$ of size m and V s.t. $\mathcal{K}$=range(V),

$$h(\omega) \approx cV(V^*AV - i\omega I)^{-1}(V^*b)$$

Next:

Classical benchmark experiment with Standard, Shift-invert and Extended Krylov

An example: CD Player, $|h(\omega)| = |C_{i,:}(A - i\omega I)^{-1} B_{:,j}|$



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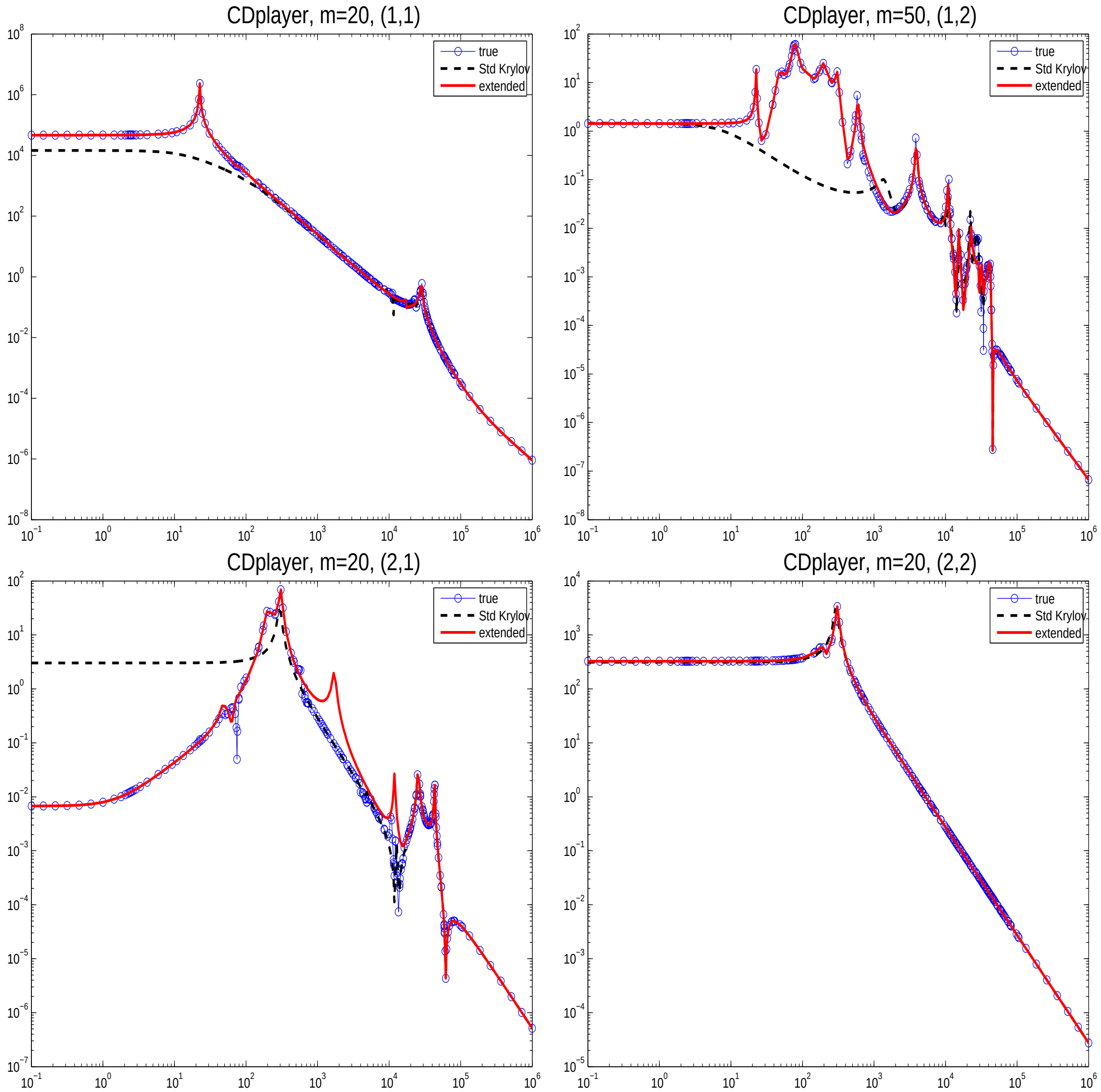


Rational Krylov Subspace Method. Choice of poles

$$K_m(A, B, \mathbf{s}) = \text{span}\{(A - s_1 I)^{-1} B, (A - s_2 I)^{-1} B, \dots, (A - s_m I)^{-1} B\}$$

cf. General discussion in Antoulas, 2005.

Various attempts:

- Gallivan, Grimme, Van Dooren (1996–, ad-hoc poles)
- Penzl (1999-2000, ADI shifts - preprocessing, Ritz values)
- ....
- Sabino (2006 - tuning within preprocessing)

- IRKA – Gugercin, Antoulas, Beattie (2008)

A new adaptive choice of poles for RKSM

$$K_m(A, b, \mathbf{s}) = \mathrm{span}\{(A - s_1 I)^{-1} b, (A - s_2 I)^{-1} b, \ldots, (A - s_m I)^{-1} b\}$$

$\mathbf{s} = [s_1, \ldots, s_m]$ to be chosen sequentially

The fundamental idea: Assume you wish to solve

$$(A - sI)x = b$$

with a Galerkin procedure in $K_m(A, b, \mathbf{s})$. Let V_m be orth. basis.
The residual satisfies:

$$b - (A - sI)x_m = \frac{r_m(A)b}{r_m(s)}, \qquad r_m(z) = \prod_{j=1}^{m} \frac{z - \lambda_j}{z - s_j}$$

with $\lambda_j = \mathrm{eigs}(V_m^* A V_m)$. Moreover,

$$\|r_m(A)b\| = \min_{\theta_1, \ldots, \theta_m} \| \prod_{j=1}^{m} (A - \theta_j I)(A - s_j I)^{-1} b \|$$

A new adaptive choice of poles for RKSM. Cont'd

$$r_m(z) = \prod_{j=1}^{m} \frac{z - \lambda_j}{z - s_j}, \qquad \lambda_j = \text{eigs}(V_m^* A V_m)$$

For A symmetric:

$$s_{m+1} := \arg \left(\max_{s \in [-\lambda_{\max}, -\lambda_{\min}]} \frac{1}{|r_m(s)|} \right)$$

$[\lambda_{\min}, \lambda_{\max}] \approx \text{spec}(A)$ (Druskin, Lieberman, Zaslavski (SISC 2010))

For A nonsymmetric:

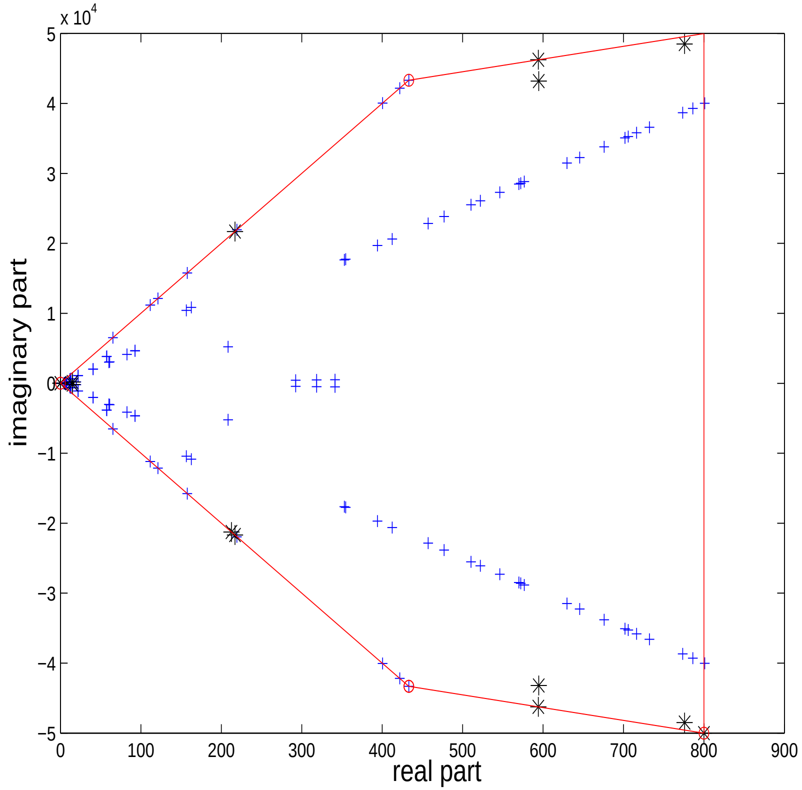
$$s_{m+1} := \arg \left(\max_{s \in \partial \mathcal{S}_m} \frac{1}{|r_m(s)|} \right)$$

where $\mathcal{S}_m \subset \mathbb{C}^+$ approximately encloses the eigenvalues of $-A$

Example of $\mathcal{S}_m$. CD Player, $m = 12$

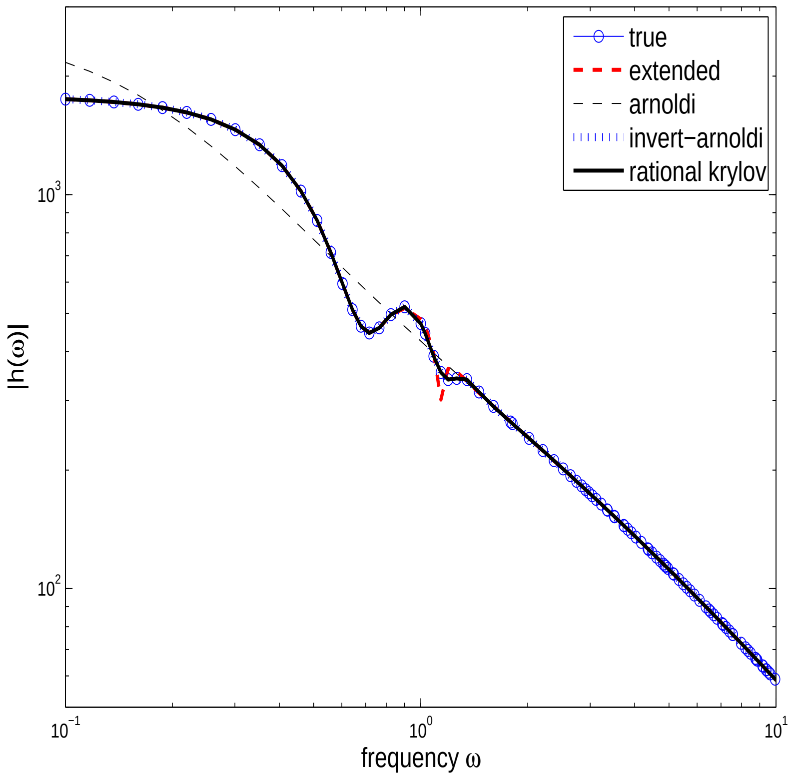
$\mathcal{S}_m$: encloses mirrored current Ritz values: -eigs$(V_m^* A V_m)$

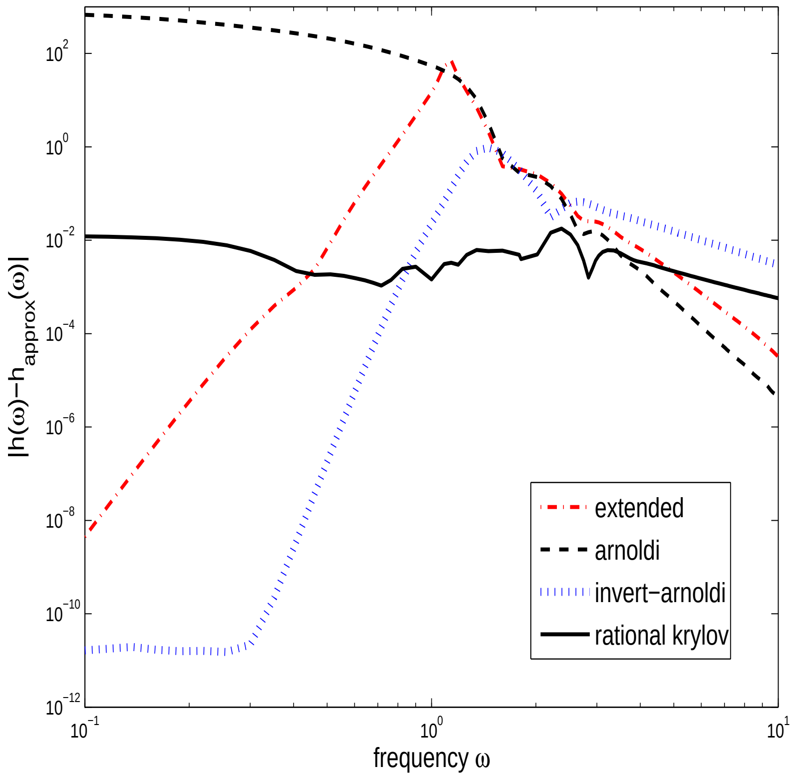
and initial estimates: $s_1^{(0)} = 0.1$, $s_{2,3}^{(0)} = 900 \pm i5 \cdot 10^4$



$*$ poles $\quad +$ -eigs(A) $\quad$ —o— $\partial\mathcal{S}_m$

Transfer function evaluation. EADY Data set



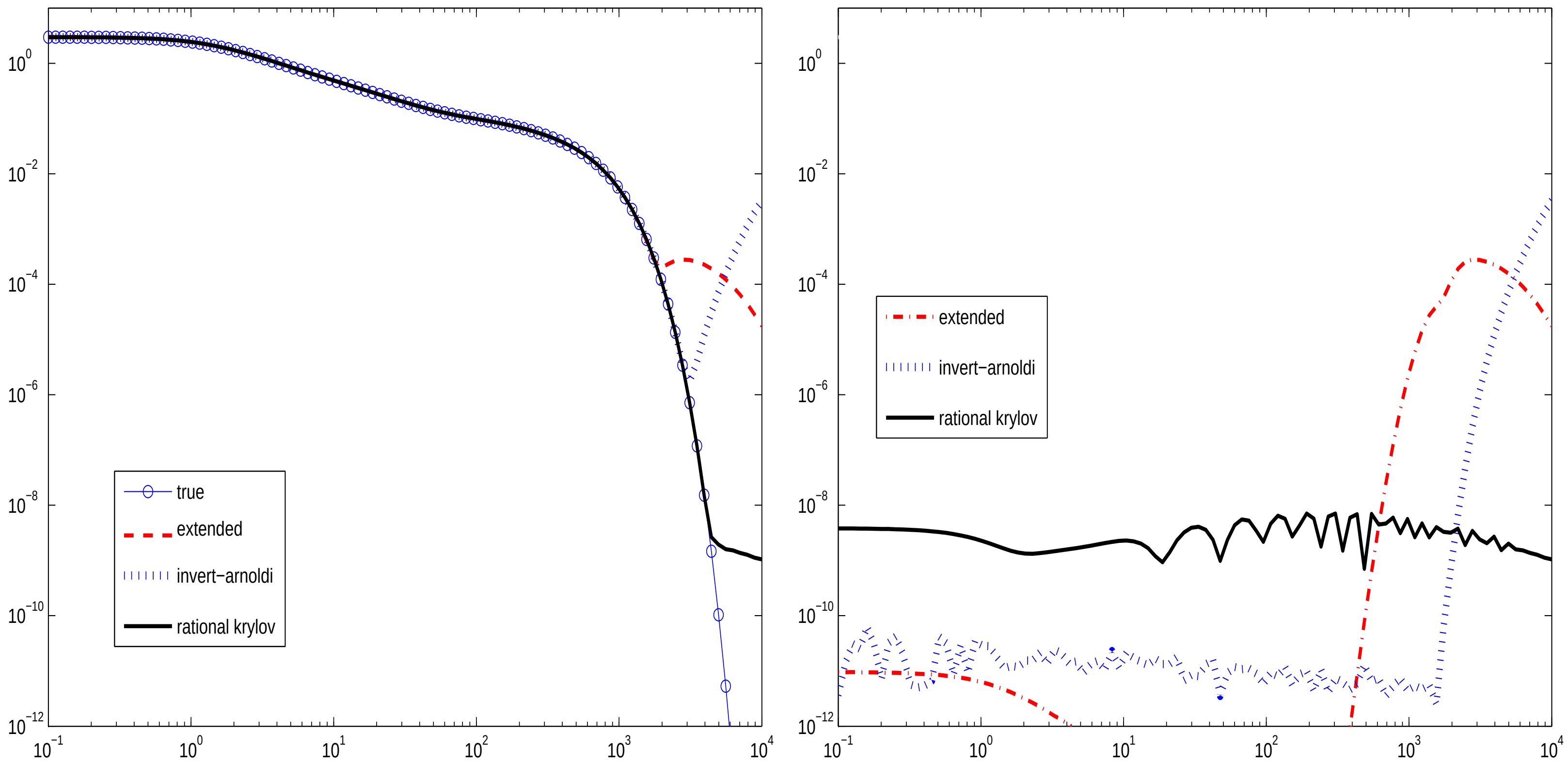


$m = 20$. A of size 598 (nonsym),

$s_1^{(0)} = \|A\|/\mathrm{condest(A)}$, $s_{2,3}^{(0)} \approx \arg(\max \Re(\mathrm{eigs}(A)))$

Transfer function evaluation. Flow Data set

$|h(\omega)|$ $\qquad$ $|h(\omega) - h_{approx}(\omega)|$



$m = 80$. A, E of size 9669 (nonsym) $s_1^{(0)} = \|A\|/(\text{condest(A)}\|E\|_F)$,
$s_2^{(0)} \approx \arg(\max \Re(\text{eigs}(A)))$ (all real poles)

Comparison with optimal (a-priori) theoretical shifts. A sym

Equidistributed nested sequence of real shifts (EDS)

(from classical Zolotaryov sol'n)

$\Rightarrow$ asymptotically optimal rational space for $i\mathbb{R}$

Rate for the L_∞ error of $h(\omega)$:

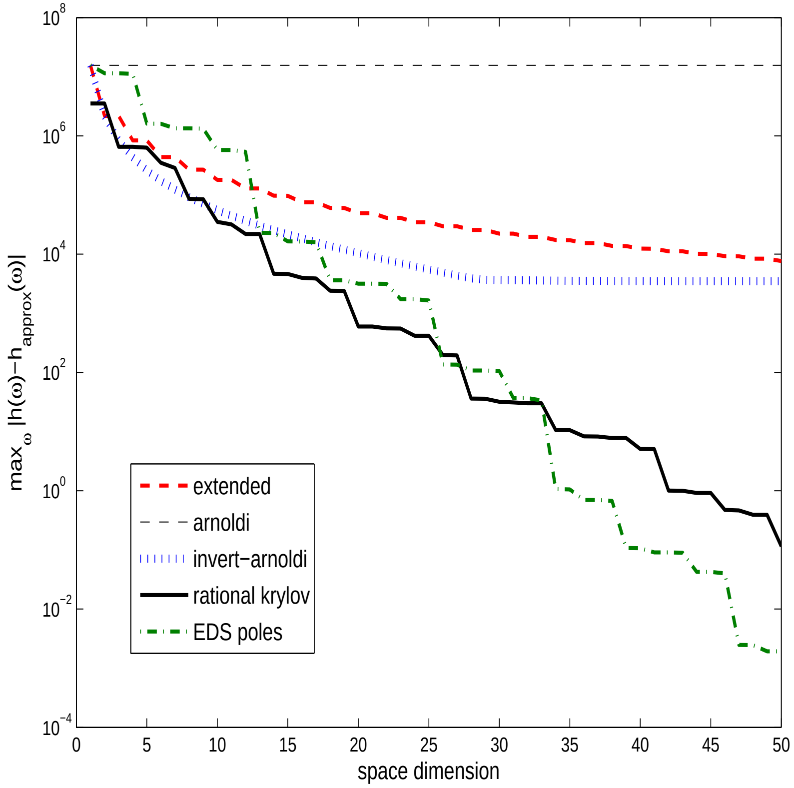
$$O\left[\exp\left(-\frac{\pi^2 m(1+o(1))}{2\log\frac{4\lambda_{\max}}{\lambda_{\min}}}\right)\right], \quad \text{for } \frac{\lambda_{\max}}{\lambda_{\min}} \gg 1$$

Druskin, Knizhnerman, Zaslavsky (SISC 2009)

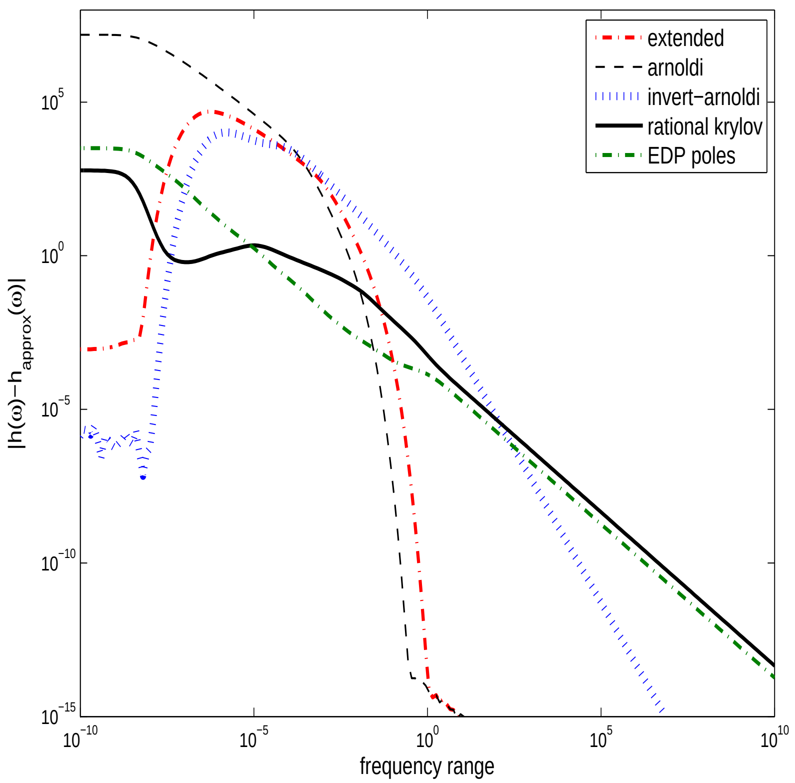
Comparison with optimal (a-priori) theoretical shifts. Cont'd

$A \in \mathbb{R}^{900\times 900}$: Diagonal matrix with log-uniformly distributed values in $[-1, -3.3164\, 10^{-9}]$

$\|h(\omega) - h_m(\omega)\|_\infty$



$|h(\omega) - h_{approx}(\omega)|$ $(m = 20)$



The Lyapunov matrix equation

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

Approximation by projection: K of dim. m, V_m orthonormal basis.
$X \approx X_m = V_m Y V_m^\top$

$$V_m^\top A V_m Y + Y V_m^\top A^\top V_m + V_m^\top b b^\top V_m = 0$$

Connection to Rational functions:

$$X = \int_{\mathbb{R}} x(\omega) x(\omega)^* d\omega \qquad \text{with} \quad x(\omega) = (A - \omega i I)^{-1} b$$

Approximation by projection

$X \approx X_m = V_m Y V_m^\top$ with

$$(V_m^\top A V_m) Y + Y (V_m^\top A V_m)^\top + (V_m^\top b)(V_m^\top b)^\top = 0$$

Some technical issues:

- $K_m(A, b, \mathbf{s}) = \text{span}\{b, (A - s_2 I)^{-1} b, \ldots, \prod_{j=2}^{m} (A - s_j I)^{-1} b\}$ (includes b)
- All real poles (all real arithmetic work)
- Cheap computation of $V_m^\top A V_m$ at each iteration m $(K_m(A, b, \mathbf{s}) \subseteq K_{m+1}(A, b, \mathbf{s}))$
- Cheap computation of the residual norm

$$\|R_m\| = \|A X_m + X_m A^\top + b b^\top\|$$

- Cheap factorized form of solution $X_m = X_{\hat{m}} := Z_{\hat{m}} Z_{\hat{m}}^\top$, $\hat{m} \le m$

Some numerical experiments

Competitors:

- ADI – problem: computation of parameters
- Extended Krylov Subspace method – outperforms ADI in general

$$\mathbf{EK}_m(A, b) = K_m(A, b) + K_m(A^{-1}, A^{-1}b)$$

Comparison measures:

- Efficiency (CPU time)
- Memory (space dimension)
- Rank of solution

The RAIL (symmetric) data set

n		Rational space direct	Extended space direct		
1357	CPU time (s)	0.84	0.36		
	dim. Approx. Space	21	64		
	Rank of Solution	21	47		
20209	CPU time (s)	11.19	10.97		
	dim. Approx. Space	25	124		
	Rank of Solution	25	75		
79841	CPU time (s)	51.54	73.03		
	dim. Approx. Space	26	168		
	Rank of Solution	26	103		

The RAIL (symmetric) data set

n		Rational space direct	Extended space direct	Rational space iterative	Extended space iterative
1357	CPU time (s)	0.84	0.36	0.96	1.60
	dim. Approx. Space	21	64	21	68
	Rank of Solution	21	47	21	45
20209	CPU time (s)	11.19	10.97	25.31	201.94
	dim. Approx. Space	25	124	25	126
	Rank of Solution	25	75	25	75
79841	CPU time (s)	51.54	73.03	189.48	2779.95
	dim. Approx. Space	26	168	26	170
	Rank of Solution	26	103	26	98

Inner solves: PCG with IC(10^{-2})

More Tests: two nonsymmetric problems

n		Rational space direct	Extended space direct	Rational space iterative	Extended space iterative
9669	CPU time (s)	3.16	3.06	3.01	9.95
	dim. Approx. Space	16	36	16	36
	Rank of Solution	16	24	16	24
20082	CPU time (s)	59.99	45.84	13.01	25.28
	dim. Approx. Space	15	26	15	26
	Rank of Solution	15	22	15	22

Convective thermal flow problems (FLOW, CHIP data sets)

$\star$ All real shifts used

Conclusions and outlook

- Adaptive procedure makes Rational Krylov subspace appealing
- Competitive in terms of both reduction space and CPU time
- Balanced Truncation?

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References:

⋆ *V. Simoncini, A new iterative method for solving large-scale Lyapunov matrix equations SIAM J. Scient. Computing, v.29, n.3 (2007), pp. 1268-1288*

⋆ *V. Simoncini, The Extended Krylov subspace for parameter dependent systems Applied Num. Math. v.60 n.5 (2010) 550-560.*

⋆ *V. Druskin and V. Simoncini, Adaptive rational Krylov subspaces for large-scale dynamical systems pp.1-20, August 2010. (Under revision)*