GAMM Anual Meeting
Novi Sad, March 20th 2013

Recent advances in low rank ADI for Lyapunov equations

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joint work with
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Outline

1. Low Rank ADI Basics
2. Low Rank Factors of Residuals
3. Adaptive ADI Shift Computation
4. Numerical Experiments

Low Rank ADI Basics

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Low Rank Solution of Lyapunov Equations

Lyapunov equation

Consider

$$FX + XF^T = -GG^T$$

with $F \in \mathbb{R}^{n \times n}$ Hurwitz, $G \in \mathbb{R}^{n \times m}$, $m \ll n$.

Goal: $$X = ZZ^H$$

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Low-rank factor ADI iteration (LR-ADI)

[Penzl '99, Benner/Li/Penzl '08]

$$V_1 = (F + p_1 I)^{-1} G, \qquad V_j = \left[I - (p_j + \overline{p_{j-1}})(F + p_j I)^{-1}\right] V_{j-1},$$

$$Z_1 := \sqrt{-2\,\mathrm{Re}\,(p_1)}\, V_1, \qquad Z_j := [Z_{j-1},\ \sqrt{-2\,\mathrm{Re}\,(p_j)}\, V_j].$$

Low Rank ADI Basics

Shift Parameters

Optimal shift parameters

For J ADI iterations, the optimal shift parameters solve the rational minmax problem

$$\min_{p_1,\ldots,p_J \subset \mathbb{C}_-} \left(\max_{1 \leq \ell \leq n} \left| \prod_{j=1}^{J} \frac{\overline{p_j} - \lambda_\ell}{p_j + \lambda_\ell} \right| \right), \qquad \lambda_\ell \in \Lambda(F).$$

(sub-)optimal shifts [Wachspress et al ~'95]

Optimal number J of shifts and their location computable for a given error tolerance for real spectra. $\rightsquigarrow$ suboptimal for $\Lambda(F) \subset \mathbb{C}$.

Heuristic *Penzl* shifts [Penzl '99]

Since λ_ℓ not easily available in large-scale setting, take small numbers of Ritz values of F and F^{-1} (generated with Arnoldi) instead.

Low Rank ADI Basics

Stopping Criteria

Relative Change of Z:

$$\frac{\left|\left|\sqrt{-2\,\mathrm{Re}\,(p_j)}V_j\right|\right|_F}{\left|\left|Z_j\right|\right|_F} \leq tol$$

Low Rank ADI Basics

Stopping Criteria

Relative Change of Z:

$$\frac{\left|\left|\sqrt{-2\,\mathrm{Re}\,(p_j)}V_j\right|\right|_F}{||Z_j||_F} \leq tol$$

$$\mathcal{L}\,(Y) := FY + YF^T + GG^T$$

Residual Based Stopping

- $\left|\left|\mathcal{L}(ZZ^T)\right|\right|_F$ computed via clever QR updates [Penzl'99]
- $\left|\left|\mathcal{L}(ZZ^T)\right|\right|_2 = \lambda_{\max}(\mathcal{L}(ZZ^T))$ apply Arnoldi/Lanczos [S. et al '09-]

Low Rank Factors of Residuals

Low Rank Factors of Residuals

Equivalence of Lyapunov and Stein Equations

e.g.[Hylla '10]

$$FX + XF^T = -GG^T \quad \overset{p\in\mathbb{C}_{<0}}{\Longleftrightarrow} \quad X = F_p X F_p^H - 2\,\mathrm{Re}\,(p) G_p G_p^H$$

Here: $F_p := (F - \overline{p}I)(F + pI)^{-1}$ and $G_p := (F + pI)^{-1} G$

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And for the ADI iterates : $X_j = F_{p_j} X_{j-1} F_{p_j}^H - 2\,\mathrm{Re}(p_j) G_{p_j} G_{p_j}^H$

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Then:

$$\begin{aligned}
\mathcal{L}(X_j) &= FX_j + X_j F^T + GG^T \\
&= F\,(X_j - X)+(X_j - X)\,F^T \\
&= \cdots = \left(\prod_{i=1}^{j} F_{p_i}\right) GG^T \left(\prod_{i=1}^{j} F_{p_i}\right)^H \\
&= W_j W_j^H.
\end{aligned}$$

Low Rank Factors of Residuals

Rank and Computability of the Residual Factor

[Benner/Kürschner/S.'13]

$$\mathcal{L}(X_j) = W_j W_j^H \quad \text{for} \quad W_j = \left(\prod_{i=1}^{j} F_{p_i} \right) G$$

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$$\begin{aligned}
V_j &= \left[I - (\overline{p_{j-1}} + p_j)(F + p_j I)^{-1} \right] V_{j-1} \\
&= (F - \overline{p_{j-1}} I)(F + p_j I)^{-1} V_{j-1} \\
&= (F - \overline{p_{j-2}} I)\, (F + p_{j-1} I)^{-1} (F - \overline{p_{j-1}} I)\, (F + p_j I)^{-1} V_{j-2} \\
&= (F - \overline{p_{j-2}} I)\, F_{p_{j-1}}\, (F + p_j I)^{-1} V_{j-2} \\
&= \cdots = (F + p_j I)^{-1} \left(\prod_{i=1}^{j-1} F_{p_i} \right) G.
\end{aligned}$$

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$$= \cdots = (F + p_j I)^{-1} \left(\prod_{i=1}^{j-1} F_{p_i}\right) G.$$

$$W_j = \left(\prod_{i=1}^{j} F_{p_i}\right) G = (F - \overline{p_j} I)\,(F + p_j I)^{-1} \left(\prod_{i=1}^{j-1} F_{p_i}\right) G$$

Low Rank Factors of Residuals

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$$W_j = (F - \overline{p_j} I) V_j$$

Low Rank Factors of Residuals

Rank and Computability of the Residual Factor

[Benner/Kürschner/S.'13]

$$W_j = (F - \overline{p_j} I)\, V_j$$

Moreover:

$$\begin{aligned} V_j &= (F + p_j I)^{-1} (F - \overline{p_{j-1}} I)\, V_{j-1} \\ &= (F + p_j I)^{-1}\, W_{j-1} \end{aligned}$$

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$$\begin{aligned} W_j &= (F - \overline{p_j} I)\, V_j = (F - \overline{p_j} I)(F + p_j I)^{-1}\, W_{j-1} \\ &= \left(I - (p_j + \overline{p_j})(F + p_j I)^{-1}\right) W_{j-1} \\ &= W_{j-1} - 2\,\mathrm{Re}\,(p_j) V_j \end{aligned}$$

The latter result was independently derived from a Krylov subspace recurrence perspective in

[Wolf/Panzer/Lohmann '13]

Low Rank Factors of Residuals

A New LR-ADI Formulation [Benner/Kürschner/S.'13]

Algorithm 1 LR-ADI Re-Formulation

Input: F,G in $FX + XF^T = -GG^T$, and proper shifts p_j, $(j = 1, \dots, J)$

Output: Z with $X \approx ZZ^H$

1: $Z = []$
2: $W_0 = G$
3: $\ell = 1$
4: **while** $(\left|\left|W_{\ell-1}^H W_{\ell-1}\right|\right| > tol$ **and** $\ell \leq J)$ **do**
5: $\quad V_\ell = (F + p_\ell I)^{-1} W_{\ell-1}$
6: $\quad W_\ell = W_{\ell-1} - 2\,\mathrm{Re}\,(p_\ell) V_\ell$
7: $\quad Z = \left[Z,\ \sqrt{-2\,\mathrm{Re}\,(p_\ell)} V_\ell\right]$
8: $\quad \ell++$
9: **end while**

Low Rank Factors of Residuals

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7: $\quad Z = \left[Z,\ \sqrt{-2\,\mathrm{Re}\,(p_\ell)} V_\ell\right]$
8: $\quad \ell{+}{+}$
9: **end while**

Note:
$\left\|W_{\ell-1} W_{\ell-1}^H\right\|_{2/F} = \left\|W_{\ell-1}^H W_{\ell-1}\right\|_{2/F}$
and $W_{\ell-1}^H W_{\ell-1}$ inner product
$\rightsquigarrow m \times m \equiv$ small

Adaptive ADI Shift Computation

Adaptive ADI Shift Computation

Basic Idea

Optimal shift parameters

For J ADI iterations, the optimal shift parameters solve the rational minmax problem

$$\min_{p_1,\ldots,p_J \subset \mathbb{C}_-} \left(\max_{1 \leq \ell \leq n} \left| \prod_{j=1}^{J} \frac{\overline{p_j} - \lambda_\ell}{p_j + \lambda_\ell} \right| \right), \qquad \lambda_\ell \in \Lambda(F).$$

- If $\Lambda(F)$ is complex: Good shifts require expert knowledge.
- The min-max-problem is solved with respect to $\Lambda(F) \rightsquigarrow \mathbb{R}^n$.
- Should we not restrict to $\mathrm{colspan}\,(Z)$? How?

Adaptive ADI Shift Computation

The New Shift Strategy

[Hund '12]

Additional assumption: $F + F^T < 0$

Then: $\Lambda(U^T F U) \subset \mathbb{C}_{<0}$ for any $U \in \mathbb{R}^{n \times k}$ orthogonal and $k \leq n$.

Bendixsons Theorem

Idea: LR-ADI converges for all proper shifts in $\mathbb{C}_{<0}$.

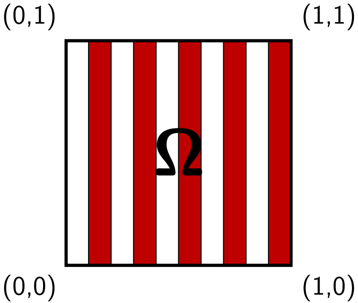
Adaptive Shift Strategy

1. $U = \mathtt{orth}(G)$
2. $p_i = \lambda_i(U^T F U)$ for all $i = 1, \ldots, m$
3. after m LR-ADI steps:
4. $U = \mathtt{orth}(V_m)$ goto 2

Numerical Experiments

Numerical Experiments

FDM discretized convection diffusion equation $n = 10\,000$, $m = 5$ [HUND '12]



- Dirichlet boundary conditions on $\Gamma = \partial\Omega$.
- Centered finite differences,
- 100 equidistant nodes in each direction.
- 5 input parameters (1 per red stripe)

$$\dot{x}(t) = -\Delta x(t) + v.\nabla x(t) + f(\xi, u(t))$$

ADI Settings:

- normalized residual tolerance 10^{-10},
- 15 Penzl shifts (from 25 large/small Ritz values)
- Wachspress (10 Arnoldi steps for F/F^{-1})

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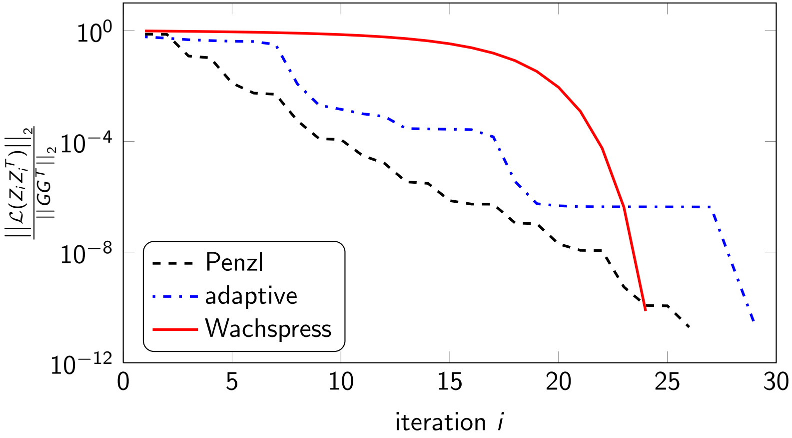

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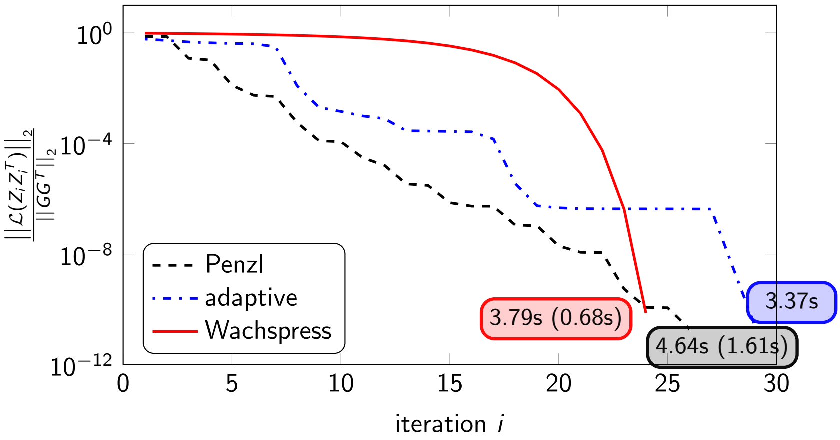
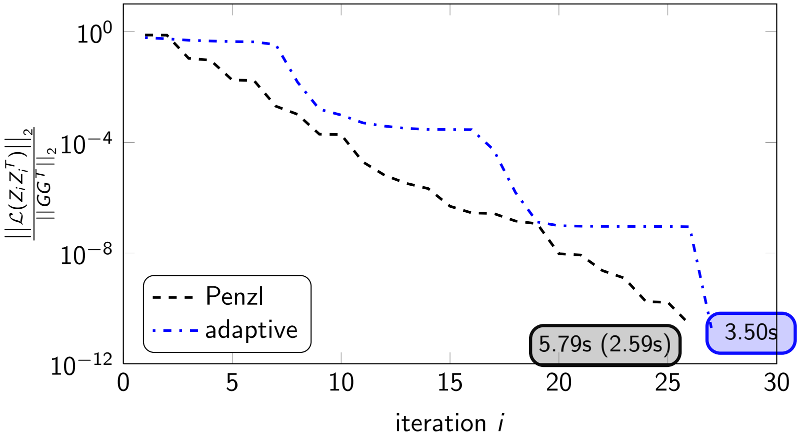


Numerical Experiments

FDM discretized convection diffusion equation $n = 10\,000$, $m = 5$

$$\dot{x}(t) = -\Delta x(t) + 10\xi_2\, \partial_{\xi_2} x(t) + f(u(t))$$



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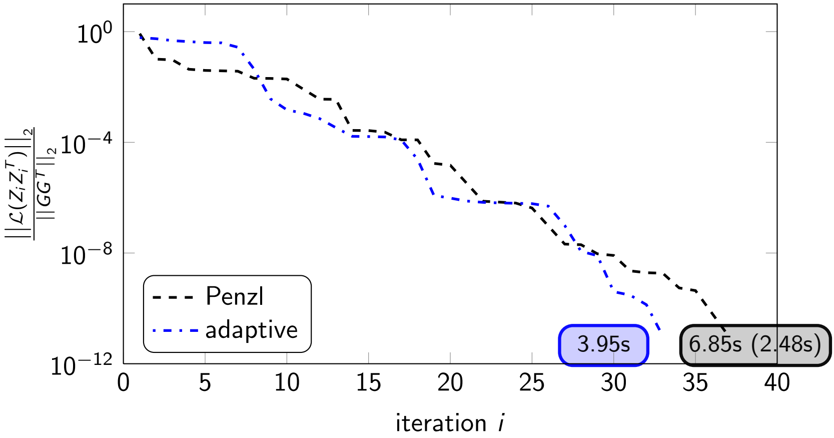

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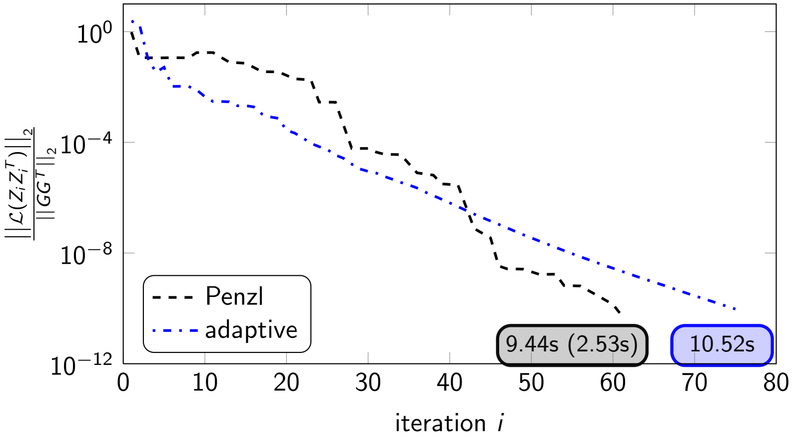


Numerical Experiments

Index-1 Power Systems Models

e.g.[FREITAS/ROMMES/MARTINS '08]

Now: Index-1 differential algebraic systems ⇝

$$FXE^T + EXF^T = -GG^T,$$

where:

$$E = \begin{bmatrix} I_s & 0 \\ 0 & 0 \end{bmatrix}, \qquad F = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}, \qquad G = \begin{bmatrix} G_1 \\ G_2 \end{bmatrix}$$

Idea: Implicitly Apply LR-ADI to the Schur complement form, i.e.,

$$\tilde{F}X + X\tilde{F}^T = -\tilde{G}\tilde{G}^T,$$

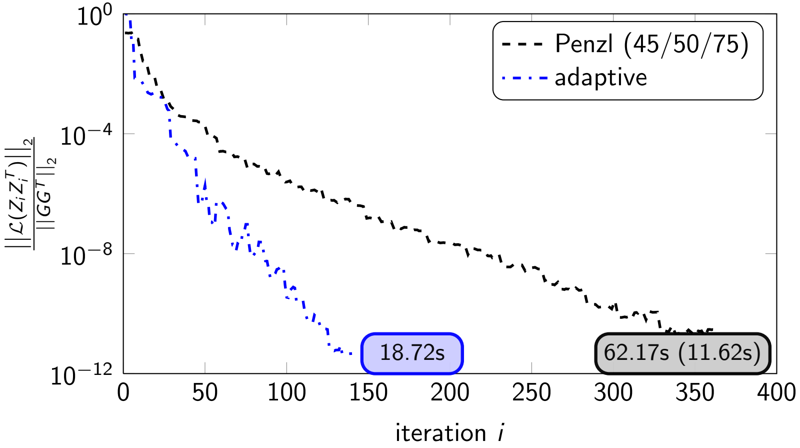
where

$$\tilde{F} = F_{11} - F_{12}F_{22}^{-1}F_{21}, \qquad \tilde{G} = G_1 - F_{12}F_{22}^{-1}G_2.$$

Numerical Experiments

Index-1 Power Systems Models e.g.[Freitas/Rommes/Martins '08]

BIPS_07[1] with $n = 21\,128$, $s = 3084$, $m = 4$



[1] https://sites.google.com/site/rommes/software

Conclusions

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- Adaptive shifts automatize the algorithm and remove required expert knowledge in selecting "good" shifts.

Thank you for your attention! Questions?