Verfahren für große dünnbesetzte Matrixgleichungen

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Seminar: Algebraische Matrixgleichungen WS 09/10

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Outline

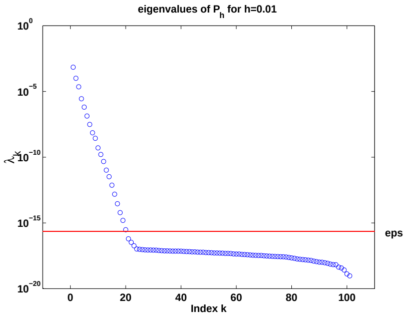
Motivation

Why use Low Rank Approximation?

The spectrum of an AREs solution

Motivating Example

- Linear 1D heat equation with point control.
- $\Omega = [0,1]$.
- FEM discretization using linear B-splines.
- h=0.01.



$$X = X^T \geq 0 \Longrightarrow X = ZZ^T = \sum_{k=1}^{n} \lambda_k z_k z_k^T \approx \sum_{k=1}^{r} \lambda_k z_k z_k^T = Z_{(r)} Z_{(r)}^T.$$

Low Rank Solvers for Lyapunov Equations

Low Rank Solvers for Lyapunov Equations

(G-)LRCF-ADI

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

ADI Iteration for the Lyapunov Equation (LE) [WACHSPRESS '88]

For $j = 1, \ldots, J$

$$\begin{aligned} X_0 &= 0 \\ (F + p_j I)X_{j-\frac{1}{2}} &= -GG^T - X_{j-1}(F^T - p_j I) \\ (F + p_j I)X_j^T &= -GG^T - X_{j-\frac{1}{2}}^T(F^T - p_j I) \end{aligned}$$

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Rewrite as one step iteration and factorize $X_i = Z_i Z_i^T$, $i = 0, \dots, J$

$$\begin{aligned} Z_0 Z_0^T &= 0 \\ Z_j Z_j^T &= -2p_j (F + p_j I)^{-1} G G^T (F + p_j I)^{-T} \\ &\quad + (F + p_j I)^{-1}(F - p_j I) Z_{j-1} Z_{j-1}^T (F - p_j I)^T (F + p_j I)^{-T} \end{aligned}$$

Low Rank Solvers for Lyapunov Equations

(G-)LRCF-ADI

$$Z_j = [\sqrt{-2p_j}(F + p_j I)^{-1}G,\ (F + p_j I)^{-1}(F - p_j I)Z_{j-1}]$$

[Penzl '00]

Low Rank Solvers for Lyapunov Equations

(G-)LRCF-ADI

$$Z_j = [\sqrt{-2p_j}(F + p_j I)^{-1} G,\ (F + p_j I)^{-1}(F - p_j I) Z_{j-1}]$$

[Penzl '00]

Observing that $(F - p_i I)$, $(F + p_k I)^{-1}$ commute, we rewrite Z_J as

$$Z_J = [z_J,\ P_{J-1} z_J,\ P_{J-2}(P_{J-1} z_J),\ \ldots,\ P_1(P_2 \cdots P_{J-1} z_J)],$$

[J. R. Li/White '02]

where

$$z_J = \sqrt{-2p_J}(F + p_J I)^{-1} G$$

and

$$P_i := \frac{\sqrt{-2p_i}}{\sqrt{-2p_{i+1}}} \left[I - (p_i + p_{i+1})(F + p_i I)^{-1} \right].$$

Low Rank Solvers for Lyapunov Equations

(G-)LRCF-ADI

Algorithm 1 Low-rank Cholesky factor ADI iteration (LRCF-ADI) [Penzl '97/'00, J. R. Li/White '99/'02, Benner/J. R. Li/Penzl '99/'08]

Input: F, G defining $FX + XF^T = -GG^T$ and shifts $\{p_1, \dots, p_{i_{max}}\}$
Output: $Z = Z_{i_{max}} \in \mathbb{C}^{n \times t_{i_{max}}}$, such that $ZZ^H \approx X$

1: $V_1 = \sqrt{-2\,\mathrm{Re}\,(p_1)}(F + p_1 I)^{-1} G$
2: $Z_1 = V_1$
3: **for** $i = 2, 3, \dots, i_{max}$ **do**
4: $\quad V_i = \sqrt{\mathrm{Re}\,(p_i)/\,\mathrm{Re}\,(p_{i-1})}(V_{i-1} - (p_i + \overline{p_{i-1}})(F + p_i I)^{-1} V_{i-1})$
5: $\quad Z_i = [Z_{i-1} \;\; V_i]$
6: **end for**

Low Rank Solvers for Lyapunov Equations

(G-)LRCF-ADI

Algorithm 2 Generalized Low-rank Cholesky factor ADI iteration (G-LRCF-ADI) [Benner '04, Benner/S. '09, S. '09]

Input: E, F, G defining $FXE^T + EXF^T = -GG^T$ and shifts $\{p_1, \ldots, p_{i_{max}}\}$
Output: $Z = Z_{i_{max}} \in \mathbb{C}^{n \times t_{i_{max}}}$, such that $ZZ^H \approx X$

1: $V_1 = \sqrt{-2\,\mathrm{Re}\,(p_1)}(F + p_1 E)^{-1} G$
2: $Z_1 = V_1$
3: **for** $i = 2, 3, \ldots, i_{max}$ **do**
4: $\quad V_i = \sqrt{\mathrm{Re}\,(p_i) / \mathrm{Re}\,(p_{i-1})}(V_{i-1} - (p_i + \overline{p_{i-1}})(F + p_i E)^{-1} E V_{i-1})$
5: $\quad Z_i = [Z_{i-1} \;\; V_i]$
6: **end for**

Low Rank Solvers for Lyapunov Equations

Krylov Subspace Based Solvers for Lyapunov Equations

Consider Schur/singular value decomposition $X = U\Sigma U^T$,
$U \in \mathbb{R}^{n\times n}$, $U^TU = I$, $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_n)$ and $|\sigma_1| \geq |\sigma_2| \geq \dots \geq |\sigma_n|$.
The best rank-m Frobenius-norm approximation to X is thus given by

$$X_m := U \begin{bmatrix} \Sigma_m & 0 \\ 0 & 0 \end{bmatrix} U^T = U_m \Sigma_m U_m^T.$$

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Krylov Projection Idea [Saad '90, Jaimoukha/Kasenally '94]

Solve

$$(U_m^T F U_m) Y_m + Y_m (U_m^T F^T U_m) = -U_m^T G G^T U_m, \quad (1)$$

on *colspan*(U_m) and get X_m as

$$X_m = U_m Y_m U_m^T.$$

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Solve

$$F_m Y_m + Y_m F_m^T = G_m G_m^T, \qquad F_m \in \mathbb{R}^{m\times m},\ m \ll n \tag{1}$$

on *colspan*(U_m) and get X_m as

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$$F_m Y_m + Y_m F_m^T = G_m G_m^T, \qquad F_m \in \mathbb{R}^{m\times m},\ m \ll n \tag{1}$$

on *colspan*(U_m) and get X_m as

$$X_m = U_m C_m C_m^T U_m^T \quad \text{where } Y_m = C_m C_m^T.$$

Low Rank Solvers for Lyapunov Equations

Krylov Subspace Based Solvers for Lyapunov Equations

Algorithm 3 Basic Krylov Subspace Method for the Lyapunov Equation

Input: F,G defining $FX + XF^T = -GG^T$, an initial Krylov subspace $\mathcal{V}$, e.g., $\mathcal{V} = \mathcal{K}_p(F, G)$ with orthogonal basis $V \in \mathbb{C}^{n\times p}$.
Output: $Z \in \mathbb{C}^{n\times t}$, such that $ZZ^H \approx X$

repeat
  if not first step **then**
    increase dimension of $\mathcal{V}$ and update V.
  end if
  Solve the "small" LE for $\tilde{Z}$ with a classical solver:

$$(V^T FV)\tilde{Z}\tilde{Z}^T + \tilde{Z}\tilde{Z}^T(V^T F^T V) = -V^T GG^T V,$$

  Lift $\tilde{Z}$ to the full space: $Z = U\tilde{Z}$
until res(Z)$<$ TOL

Low Rank Solvers for Lyapunov Equations

Krylov Subspace Based Solvers for Lyapunov Equations

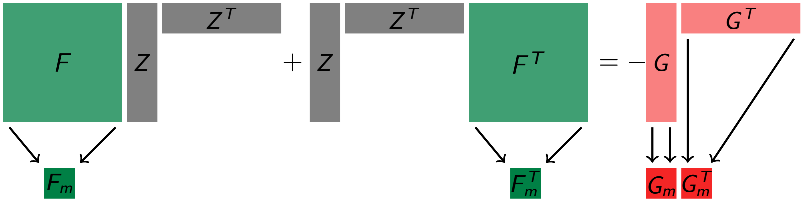
$$F\,Z\,Z^T + Z\,Z^T\,F^T = -G\,G^T$$

Legend:

new factor original matrix projected matrix projected Cholesky factor
old factor original rhs projected rhs

Low Rank Solvers for Lyapunov Equations

Krylov Subspace Based Solvers for Lyapunov Equations



Legend:

new factor original matrix projected matrix projected Cholesky factor
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Low Rank Solvers for Lyapunov Equations

Krylov Subspace Based Solvers for Lyapunov Equations

$$F_m \; C_m C_m^T + C_m C_m^T \; F_m^T = -G_m G_m^T$$

Legend:

new factor original matrix projected matrix projected Cholesky factor
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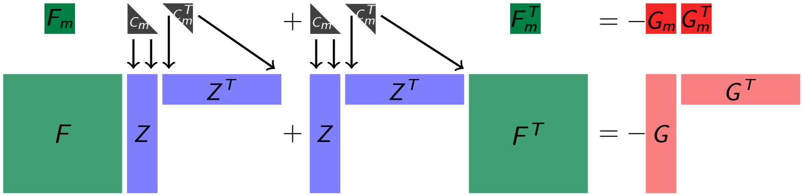

Legend:

new factor | original matrix | projected matrix | projected Cholesky factor

old factor | original rhs | projected rhs

LRCF-NM for the ARE

LRCF-NM for the ARE

Newton's Method for AREs

Consider $\mathfrak{R}(X) := C^T C + A^T X + XA - XBB^T X = 0$

Newton's Iteration for the ARE

$$\mathfrak{R}'|_X(N_\ell) = -\mathfrak{R}(X_\ell), \qquad X_{\ell+1} = X_\ell + N_\ell, \qquad \ell = 0, 1, \dots$$

where the Frechét derivative of $\mathfrak{R}$ at X is the Lyapunov operator

$$\mathfrak{R}'|_X : \quad Q \mapsto (A - BB^T X)^T Q + Q(A - BB^T X),$$

i.e., in every Newton step solve a

Lyapunov Equation [Kleinman '68]

$$(A - BB^T X_\ell)^T X_{\ell+1} + X_{\ell+1}(A - BB^T X_\ell) = -C^T C - X_\ell BB^T X_\ell.$$

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Lyapunov Equation [Kleinman '68]

$$F_\ell^T X_{\ell+1} + X_{\ell+1} F_\ell = -G_\ell G_\ell^T.$$

LRCF-NM for the ARE

Newton's Method for AREs

Consider $\mathfrak{R}(X) := C^TC + A^TXE + E^TXA - E^TXBB^TXE = 0$

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Lyapunov Equation [KLEINMAN '68]

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LRCF-NM for the ARE

Low-Rank Newton-ADI (LRCF-NM) for AREs

Factored Newton-Kleinman Iteration [Benner/J. R. Li/Penzl '99/'08]

$$F_\ell = A - BB^T X_\ell =: A - BK_\ell$$ is "sparse + low rank"

$$G_\ell = [C^T \; K_\ell^T]$$ is low rank factor

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- apply LRCF-ADI in every Newton step
- exploit structure of F_ℓ using Sherman-Morrison-Woodbury formula

$$(A - BK_\ell + p_k^{(\ell)} I_n)^{-1} = (I_n + (A + p_k^{(\ell)} I_n)^{-1} B (I_m - K_\ell (A + p_k^{(\ell)} I_n)^{-1} B)^{-1} K_\ell)(A + p_k^{(\ell)} I_n)^{-1}$$

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Low-Rank Newton-ADI (LRCF-NM) for AREs

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$$G_\ell = [C^T \ K_\ell^T] \quad \text{is low rank factor}$$

- apply LRCF-ADI in every Newton step
- exploit structure of F_ℓ using Sherman-Morrison-Woodbury formula

$$(A - BK_\ell + p_k^{(\ell)} E)^{-1} = (I_n + (A + p_k^{(\ell)} E)^{-1} B (I_m - K_\ell (A + p_k^{(\ell)} E)^{-1} B)^{-1} K_\ell)(A + p_k^{(\ell)} E)^{-1}$$

LRCF-NM for the ARE

QADI

$$(A^T - K_{j-1}^T B^T + p_j I) X_{j-\frac{1}{2}}^T = -Q - X_{j-1}^T (A - p_j I),$$
$$(A^T - K_{j-\frac{1}{2}}^T B^T + p_j I) X_j = -Q - X_{j-\frac{1}{2}} (A - p_j I).$$

LRCF-NM for the ARE

QADI

$$
\begin{aligned}
(A^T - K_{j-1}^T B^T + p_j I) X_{j-\frac{1}{2}}^T &= -Q - K_{j-1}^T R K_{j-1} - X_{j-1}^T (A - B K_{j-1} - p_j I),\\
(A^T - K_{j-\frac{1}{2}}^T B^T + p_j I) X_j &= -Q - K_{j-\frac{1}{2}}^T R K_{j-\frac{1}{2}} - X_{j-\frac{1}{2}} (A - B K_{j-\frac{1}{2}} - p_j I).
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LRCF-NM for the ARE

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\end{aligned}
$$

NK-ADI

$$
\begin{aligned}
(A^T - K_{j-1}^T B^T + p_k I) X_{k-\frac{1}{2}}^T &= -Q - K_{j-1}^T R K_{j-1} - X_{k-1}^T (A - K_{j-1}^T B^T - p_k I),\\
(A^T - K_{j-1}^T B^T + p_k I) X_k &= -Q - K_{j-1}^T R K_{j-1} - X_{k-\frac{1}{2}} (A - B K_{j-1} - p_k I).
\end{aligned}
$$

ADI Shift Parameter Choice

Min-Max-Problem

Optimal parameters solve the

min-max-problem

$$\min_{\{p_j \in \mathbb{R} | j=1,\ldots,J\} \subset \mathbb{R}} \quad \max_{\lambda \in \sigma(H), \gamma \in \sigma(V)} \left| \prod_{j=1}^{J} \frac{(p_j - \lambda)(p_j - \gamma)}{(p_j + \lambda)(p_j + \gamma)} \right| .$$

Remark

- Also known as rational Zolotarev problem since he solved it first on real intervals enclosing the spectra in 1877.
- Another solution for the real case was presented by Wachspress/Jordan in 1963.
- Wachspress and Starke presented different strategies to compute suboptimal shifts for the complex case around 1990.

ADI Shift Parameter Choice

Min-Max-Problem

Optimal parameters solve the

min-max-problem

$$\min_{\{p_j\in\mathbb{R}|j=1,\ldots,J\}\subset\mathbb{R}} \quad \max_{\lambda\in\sigma(F),} \quad \left|\prod_{j=1}^{J}\frac{(p_j-\lambda)}{(p_j+\lambda)}\right|.$$

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ADI Shift Parameter Choice

Common ADI Shift Parameter Choices

We will discuss three possible parameter choices here:

1. (sub-) optimal parameters [WACHSPRESS: ADI model problem '95] :
   - optimal for real spectra
   - Solve the min-max-problem on an elliptic functions region.
   - Computation needs knowledge of the complete spectrum of F.
   - parameters real if imaginary parts are "small"
2. heuristic parameters [PENZL: Lyapack '99]
   - use Ritz values as shifts
   - suboptimal $\Rightarrow$ convergence might be slow
   - in general complex for complex spectra
3. semi-optimal parameters: Idea: combine the advantages of these methods [BENNER/ MENSA/ S. '08: ALA2006]
   - use Arnoldi's method to approximate the outer spectrum
   - compute the (sub-)optimal real parameters for this approximation