MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Numerical Solution of Matrix Equations Arising in DSGE Models

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The Max Planck Institute (MPI) in Magdeburg

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- is dedicated to fundamental research;
- operates 84 institutes — 79 in Germany, 2 in Italy (Rome, Florence), 1 each in The Netherlands, Luxembourg, US;
- has $\sim$ 23,000 employees;
- had 18 Nobel Laureates since 1948.

"The first MPI in engineering. . . "

- founded 1998
- 4 departments (directors)
- 10 research groups
- budget $\sim$ 15 Mio. EUR
- $\sim$ 230 employees
- $\sim$ 160 scientific staff,
- doing research in
  - biotechnology
  - chemical engineering
  - process engineering
  - energy conversion
  - applied math
  - HPC

Work on Numerical Methods for Matrix Equations

Selected publications since 1993

- G. S. Ammar, P. Benner, and V. Mehrmann, *A multishift algorithm for the numerical solution of algebraic Riccati equations*, Electron. Trans. Numer. Anal., 1 (1993), pp. 33–48.
- P. Benner and R. Byers, *An exact line search method for solving generalized continuous-time algebraic Riccati equations*, IEEE Trans. Autom. Control, 43 (1998), pp. 101–107.
- P. Benner and E. S. Quintana-Ortí, *Solving stable generalized Lyapunov equations with the matrix sign function*, Numer. Algorithms, 20 (1999), pp. 75–100.
- P. Benner, *Factorized solution of Sylvester equations with applications in control*, in Proc. Intl. Symp. Math. Theory Networks and Syst. MTNS 2004, 2004.
- P. Benner, E. S. Quintana-Ortí, and G. Quintana-Ortí, *Solving stable Sylvester equations via rational iterative schemes*, J. Sci. Comp., 28 (2006), pp. 51–83.
- P. Benner, J.-R. Li, and T. Penzl, *Numerical solution of large-scale Lyapunov equations, Riccati equations, and linear-quadratic optimal control problems*, Numer. Lin. Alg. Appl., 15 (2008), pp. 755–777.
- P. Benner, R.-C. Li, and N. Truhar, *On the ADI method for Sylvester equations*, J. Comput. Appl. Math., 233 (2009), pp. 1035–1045.
- P. Benner and H. Fassbender, *On the numerical solution of large-scale sparse discrete-time Riccati equations*, Adv. Comput. Math., 35 (2011), pp. 119–147.
- P. Benner and J. Saak, *Numerical solution of large and sparse continuous time algebraic matrix Riccati and Lyapunov equations: a state of the art survey*, GAMM Mitteilungen, 36 (2013), pp. 32–52.
- P. Benner and P. Kürschner, *Computing real low-rank solutions of Sylvester equations by the factored ADI method*, Comput. Math. Appl., 67 (2014), pp. 1656–1672.
- P. Benner, P. Kürschner, and J. Saak, *Low-rank Newton-ADI methods for large nonsymmetric algebraic Riccati equations*, J. Frankl. Inst., 353 (2016), pp. 1147–1167.
- P. Benner, Z. Bujanović, P. Kürschner, and J. Saak, *RADI: A low-rank ADI-type algorithm for large scale algebraic Riccati equations*, Numer. Math., 138 (2018), pp. 301–330.

Problem: Find $X \in \mathbb{R}^{n\times n}$ such that

$$AX^2 + BX + C = 0, \qquad A, B, C \in \mathbb{R}^{n\times n}.$$

Unilateral quadratic matrix equations (UQME) arise in

- solving large-scale Dynamic Stochastic General Equilibrium (DSGE) models;
- quasi-birth-death processes;
- quadratic eigenvalue problems.

The Unilateral Quadratic Matrix Equation

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Unilateral quadratic matrix equations (UQME) arise in

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- quadratic eigenvalue problems.

Explicit formula for solution of scalar quadratic equations does not generalize to UQME, except in special situations: e.g., if $A = I_n$ *and* B, C commute, then

$$X = -\frac{1}{2}B \pm (B^2 - 4C)^{\frac{1}{2}} \qquad \text{if } B^2 - 4C \text{ has a matrix root.}$$

$\rightsquigarrow$ need numerical solution schemes!

N.J. Higham and H.M. Kim. *Numerical analysis of a quadratic matrix equation*. IMA Journal of Numerical Analysis 20(4):499–519, 2000.

The Schur Method for UQME

Theorem ([Higham/Kim 2000])

Given $A, B, C \in \mathbb{R}^{n\times n}$, consider the UQME $AX^2 + BX + C = 0.$

a) *$X \in \mathbb{R}^{n\times n}$ solves the UQME if and only if*

$$\underbrace{\begin{bmatrix} 0 & I_n \\ -C & -B \end{bmatrix}}_{=:F} \begin{bmatrix} I_n \\ X \end{bmatrix} = \underbrace{\begin{bmatrix} I_n & 0 \\ 0 & A \end{bmatrix}}_{=:G} \begin{bmatrix} I_n \\ X \end{bmatrix} X.$$

In mathematical terms, X defines an n-dimensional graph subspace of the matrix pencil $F - \lambda G$, corresponding to the eigenvalues $\Lambda(X) \subset \Lambda(F, G)$.

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Given $A, B, C \in \mathbb{R}^{n\times n}$, consider the UQME $AX^2 + BX + C = 0.$

b) *Let*

$$F = Q\Sigma Z^T, \quad G = Q\Phi Z^T, \quad \text{with } \Sigma, \Phi = \left[\diagdown \right],$$

where $Q, Z \in \mathbb{R}^{n\times n}$ are orthogonal ($Q^TQ = Z^TZ = I_n$), be the generalized Schur decomposition of $F - \lambda G$.

Then every solution $X \in \mathbb{R}^{n\times n}$ of the UQME has the form

$$X = Z_{21}Z_{11}^{-1} = Q_{11}\Sigma_{11}\Phi_{11}^{-1}Q_{11}^{-1},$$

with M_{ij} denoting the blocks in a uniform 2×2-block partitioning of M.

Note: different solutions X correspond to different orderings of the eigenvalues of $F - \lambda G$, i.e., different orderings of the diagonal elements of Σ, Φ.

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The Schur Method for UQME

The characterization of solutions leads directly to a numerical solution method for the UQME:

1. Form the $2n \times 2n$-block matrices F, G.
2. Compute the generalized Schur decomposition of $F - \lambda G$ (e.g., using the QZ algorithm in MATLAB via qz).
3. Re-order the diagonal elements/eigenvalues in the generalized Schur form as needed.
4. Solve $XZ_{11} = Z_{21}$.

Remark

As

$$\mathrm{cond}_2(Z_{11}) \leq 1 + \|X\|_2,$$

scaling $X \to X/\rho$ with $\rho \approx X$ may improve the accuracy of the solution.

+ QZ algorithm [Moler/Stewart 1973] is numerically backward stable and is implemented in LAPACK, the backbone of Intel's MKL, the MATLAB Linear Algebra kernel, etc.

B. Kågström and D. Kressner. *Multishift variants of the QZ algorithm with aggressive early deflation*. SIAM Journal on Matrix Analysis and Applications 29(1):199–227, 2008.

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- – Data access pattern and data dependencies make the QZ algorithm a serial, communication-bound algorithm.
- – Therefore, QZ algorithm is notoriously difficult to parallelize. Hence, it is not efficient on modern multicore architectures.
- \+ Recent performance improvement using block variant of QZ algorithm [Kågström/Kressner 2008], not yet included in LAPACK.

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- Uniform $(-1, 1)$ random matrices
- Compute generalized Schur decomposition only
- 2x8 core Intel Xeon Silver 4110, 192 GB RAM, Intel MKL 2018.1

Dim. n	LAPACK	KKQZ	Speed-up
5 000	873s	482s	1.81
10 000	9 630s	5 647s	1.71
15 000	27 623s	17 195s	1.61
20 000	77 935s	48 189s	1.62
25 000	141 207s	86 009s	1.64

Basic Idea: for solving UQME, only basis of subspace spanned by $\begin{bmatrix} I \\ X \end{bmatrix}$ is needed, that is, a separation of the spectrum into 2 clusters rather than a separation of all eigenvalues as in the generalized Schur decompostion.

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Therefore, need $Q, Z \in \mathbb{R}^{n\times n}$ (orthogonal) such that

$$Q(F - \lambda G)Z \quad = \quad \begin{bmatrix} F_{11} & F_{12} \\ & F_{22} \end{bmatrix} - \lambda \begin{bmatrix} G_{11} & G_{12} \\ & G_{22} \end{bmatrix}$$

A Sign Function Approach to Solving UQMEs

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i.e., block-triangular decomposition!

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This can be computed by spectral projection methods like (generalized) sign and disk function methods.

[Roberts 1971]

Definition (Matrix sign function)

Given $Z \in \mathbb{R}^{n \times n}$ with k / $n-k$ eigenvalues in the open left / right half of the complex plane and Jordan decomposition

$$Z = S \begin{bmatrix} J^- & 0 \\ 0 & J^+ \end{bmatrix} S^{-1},$$

where the Jordan blocks corresponding to the eigenvalues

- in the open left half plane are collected in $J^- \in \mathbb{C}^{k \times k}$,
- in the open right half plane are collected in $J^+ \in \mathbb{C}^{n-k \times n-k}$.

Then

$$\operatorname{sign}(Z) := S \begin{bmatrix} -I_k & 0 \\ 0 & I_{n-k} \end{bmatrix} S^{-1},$$

and $\mathrm{range}\,(I_n - \operatorname{sign}(Z))$ is the Z-invariant subspace corresponding to J^-.

Computing the matrix sign function

Applying Newton's method to $F(Z) = Z^2 - I$ with $Z_0 := Z$ yields

$$Z_0 \leftarrow Z, \quad Z_{j+1} \leftarrow \frac{1}{2c_j}(Z_j + c_j^2 Z_j^{-1}), \qquad j = 0, 1, \ldots,$$

with $\lim_{j\to\infty} Z_j = \operatorname{sign}(Z)$ and where c_j is a scaling factor accelerating convergence.

Stable Z-invariant subspace can be computed using pivoted QR decomposition of SVD applied to $I - \operatorname{sign}(Z)$.

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Application to matrix pencils $F - \lambda G$**:** apply sign function iteration implicitly to $Z := G^{-1}F$, leading to

$$F_0 \leftarrow F, \quad F_{j+1} \leftarrow \frac{1}{2c_j}(F_j + c_j^2 G F_j^{-1} G), \qquad j = 0, 1, \ldots,$$

and $\mathrm{range}\,(\lim_{j\to\infty} F_j - G)$ provides stable "deflating" subspace.

Note: Usually, $c_j = \left(\frac{|\det(Z_j)|}{|\det(Y)|}\right)^{\frac{1}{n}}$.

Algorithm 1 Generalized Sign Function Method

Input: A matrix pencil $F - \lambda G$, $F, G \in \mathbb{R}^{n \times n}$ with no eigenvalues on the imaginary axis.

Output: generalized sign function $F_\infty - \lambda G$.

1: Set $F_0 = F$, $g = |\det G|^{\frac{1}{n}}$.

2: **for** $j = 0, 1, \ldots$ until convergence **do**

3: $\quad F_j = \Pi^T LU$ $\{$*LU factorization: L/U lower/upper triangular,* Π *permutation*$\}$

4: $\quad c_j = \left(\prod_{k=1}^{n} |u_{kk}|^{\frac{1}{n}}\right) / g$.

5: $\quad$ Solve $LW = \Pi G$ by forward substitution.

6: $\quad$ Solve $UX = W$ by backward substitution.

7: $\quad F_{j+1} = \frac{1}{2c_j} F_j + \frac{c_j}{2} GX$.

8: **end for**

Set-up:

- Uniform $(-1, 1)$ random matrices
- 2x8 core Intel Xeon Silver 4110, 192 GB RAM, Intel MKL 2018.1
- sign function run to compute generalized Schur form (not block-triangular form!)

Dim. m	LAPACK	KKQZ	sign fct.	Speed-up	Error [1]
5 000	873s	482s	123s	3.91	$1.42 \cdot 10^{-11}$
10 000	9 630s	5 647s	645s	8.76	$2.69 \cdot 10^{-10}$
15 000	27 623s	17 195s	2 217s	7.75	$8.59 \cdot 10^{-13}$
20 000	77 935s	48 189s	4 838s	9.96	$7.39 \cdot 10^{-11}$
25 000	141 207s	86 009s	8 213s	10.47	$4.08 \cdot 10^{-11}$

[1] $\max\{\frac{||A-QA_sZ^T||}{||A||}, \frac{||B-QB_sZ^T||}{||B||}\}$

A Sign Function Approach to Solving UQMEs

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- Natural splitting of eigenvalues computed by (generalized) sign function is w.r.t. imaginary axis. Thus, apply sign function method to

$$\tilde{F} \leftarrow F - G = \begin{bmatrix} -I_n & I_n \\ -C & A - B \end{bmatrix}, \quad \tilde{G} \leftarrow F + G = \begin{bmatrix} I_n & I_n \\ -C & -(A + B) \end{bmatrix}.$$

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- Potential computational savings: matrix product with G:

$$\begin{aligned} \tilde{G}M &= \begin{bmatrix} I_n & I_n \\ -C & -(A + B) \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \\ &= \begin{bmatrix} M_{11} + M_{21} & M_{12} + M_{22} \\ [-N_0, 0]M_{11} - (A + B)M_{21} & [-N_0, 0]M_{12} - (A + B)M_{22} \end{bmatrix} \end{aligned}$$

Implementing this efficiently requires $4n^2(n + n_x)$ flops instead of $16n^3$; this should save $\approx 50\%$ of the operations/time per iteration!

A Sign Function Approach to Solving UQMEs

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  Implementing this efficiently requires $4n^2(n + n_x)$ flops instead of $16n^3$; this should save $\approx 50\%$ of the operations/time per iteration!
- No re-ordering needed as in Schur method!

- (Quasi-)Newton's method for $0 = Q(X) = AX^2 + BX + C$:

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- Functional iterations, e.g., Bernoulli iteration
  $$X_{k+1} = -A^{-1}(B + CX_k^{-1}).$$
  Not applicable for DSGE models, as A is singular.
- Cyclic reduction — numerical stability is not guaranteed.

Outline

The following linear matrix equations occur in the recursive solution of DSGE models using perturbation methods [HARDING '19]:

Generalized Sylvester Equation

$$A_0 Y + A Y \overline{C}_z + P_0 + P_1 \overline{C}_z = 0,$$

where

- $A, A_0 \in \mathbb{R}^{n \times n}$, $\overline{C}_z \in \mathbb{R}^{n_z \times n_z}$, $P_0, P_1 \in \mathbb{R}^{n \times n_z}$,
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- and $Y \in \mathbb{R}^{n \times n_z}$ is the unknown matrix.

This can be transformed to a smaller Sylvester equation:

Sylvester Equation

$$TZ + Z\overline{C}_z + W = 0, \qquad T, W \in \mathbb{R}^{n_z \times n_z},$$

where $Z \in \mathbb{R}^{n_z \times n_z}$ is the unknown matrix.

Sylvester equation

James Joseph Sylvester
(September 3, 1814 – March 15, 1897)

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Lyapunov equation

Alexander Michailowitsch Ljapunow
(June 6, 1857 – November 3, 1918)

$$AX + XA^T = C, \quad C = C^T.$$

Generalized Sylvester equation:

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Stein equation:

$$X - AXB = C.$$

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Stein equation:

$$X - AXB = C.$$

(Generalized) discrete Lyapunov/Stein equation:

$$EXE^T - AXA^T = C, \quad C = C^T.$$

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Note:

- Consider only regular cases, having a unique solution!
- Solutions of symmetric cases are symmetric, $X = X^T \in \mathbb{R}^{n \times n}$; otherwise, $X \in \mathbb{R}^{n \times \ell}$ with $n \neq \ell$ in general.

Bilinear Lyapunov equation/Lyapunov-plus-positive equation:

$$AX + XA^T + \sum_{k=1}^{m} N_k X N_k^T = C, \quad C = C^T.$$

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(Generalized) discrete bilinear Lyapunov/Stein-minus-positive eq.:

$$EXE^T - AXA^T - \sum_{k=1}^{m} N_k X N_k^T = C, \quad C = C^T.$$

Note: Again consider only regular cases, symmetric equations have symmetric solutions.

Exemplarily, consider the generalized Sylvester equation

$$AXD + EXB = C. \tag{1}$$

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Vectorization (using Kronecker product) $\rightsquigarrow$ representation as linear system:

$$\big(\underbrace{D^T \otimes A + B^T \otimes E}_{=:\mathcal{A}}\big)\underbrace{\mathrm{vec}(X)}_{=:x} = \underbrace{\mathrm{vec}(C)}_{=:c} \quad\Longleftrightarrow\quad \mathcal{A}x = c.$$

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Lemma

$$\Lambda(\mathcal{A}) = \{\alpha_j + \beta_k \mid \alpha_j \in \Lambda(A, E),\ \beta_k \in \Lambda(B, D)\}.$$

Hence, (1) has unique solution $\Longleftrightarrow$ $\Lambda(A, E) \cap -\Lambda(B, D) = \emptyset$.

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Example: Lyapunov equation $AX + XA^T = C$ has unique solution

$$\iff \nexists\, \mu \in \mathbb{C} \,:\, \pm\mu \in \Lambda(A).$$

Theorem (Lyapunov 1892)

Let $A \in \mathbb{R}^{n \times n}$ and consider the Lyapunov operator $\mathcal{L} : X \rightarrow AX + XA^T$. Then the following are equivalent:

(a) $\forall Y > 0$: $\exists X > 0$: $\mathcal{L}(X) = -Y$,

(b) $\exists Y > 0$: $\exists X > 0$: $\mathcal{L}(X) = -Y$,

(c) $\Lambda(A) \subset \mathbb{C}^- := \{z \in \mathbb{C} \,|\, \Re z < 0\}$, *i.e., A is (asymptotically) stable or Hurwitz.*

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The proof (c) $\Rightarrow$ (a) is trivial from the necessary and sufficient condition for existence and uniqueness, apart from the positive definiteness. The latter is shown by studying $z^H Y z$ for all eigenvectors z of A.

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Important in applications: the nonnegative case:

$$\mathcal{L}(X) = AX + XA^T = -WW^T, \quad \text{where} \quad W \in \mathbb{R}^{n\times n_W},\ n_W \ll n.$$

A Hurwitz $\Rightarrow$ $\exists$ unique solution $X = ZZ^T$ for $Z \in \mathbb{R}^{n\times n_X}$ with $1 \le n_X \le n$.

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From Lyapunov's theorem, one immediately obtains a characterization of asymptotic stability of linear dynamical systems

$$\dot{x}(t) = Ax(t). \qquad (2)$$

Theorem (Lyapunov)

The following are equivalent:

- *For (2), the zero state is asymptotically stable.*
- *The Lyapunov equation $AX + XA^T = Y$ has a unique solution $X = X^T > 0$ for all $Y = Y^T < 0$.*
- *A is Hurwitz.*

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Solving AREs by Newtons's Method

Feedback control design often involves solution of

$$A^T X + XA - XGX + H = 0, \quad G = G^T, H = H^T.$$

$\rightsquigarrow$ In each Newton step, solve Lyapunov equation

$$(A - GX_j)^T X_{j+1} + X_{j+1}(A - GX_j) = -X_j G X_j - H.$$

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Decoupling of dynamical systems, e.g., in slow/fast modes, requires solution of nonsymmetric ARE

$$AX + XF - XGX + H = 0.$$

$\rightsquigarrow$ In each Newton step, solve Sylvester equation

$$(A - X_j G)X_{j+1} + X_{j+1}(F - GX_j) = -X_j G X_j - H.$$

Also occurs in solving DSGE models, but how to compute desired solution?

Model Reduction via Balanced Truncation

For linear dynamical system

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx_r(t), \qquad x(t) \in \mathbb{R}^n$$

find reduced-order system

$$\dot{x}_r(t) = A_r x_r(t) + B_r u(t), \quad y_r(t) = C_r x_r(t), \qquad x(t) \in \mathbb{R}^r, \quad r \ll n$$

such that $\|y(t) - y_r(t)\| < \delta$.

The popular method balanced truncation requires the solution of the dual Lyapunov equations

$$AX + XA^T + BB^T = 0, \qquad A^T Y + YA + C^T C = 0.$$

Sylvester equation $AX - XB = C$ is equivalent to linear system of equations

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Possible solvers:

- Hessenberg-Schur or Bartels-Stewart method [Bartels/Stewart '72, Golub/Nash/Van Loan '79]
- Sign function method [Roberts '71, B '04]
- Krylov subspace solvers in operator from [Hochbruck, Starke, Reichel, ...]
- Block-Tensor-Krylov subspace methods with truncation [Kressner/Tobler, Bollhöfer/Eppler, B./Breiten, ...]
- Galerkin-type methods based on (extended, rational) Krylov subspace methods [Jaimoukha, Kasenally, Jbilou, Simoncini, Druskin, Knizhermann,...]
- ADI methods [Wachspress, Reichel, Li^2, Penzl, B, Saak, Kürschner, Truhar, Tomljanović...]

Sylvester Equations

Find $X \in \mathbb{R}^{n \times m}$ solving

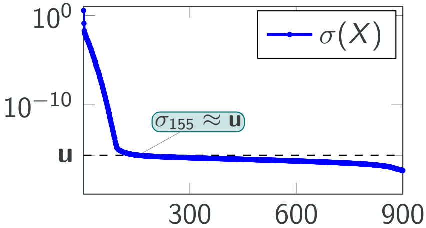
$$AX - XB = FG^T,$$

where $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{m \times m}$, $F \in \mathbb{R}^{n \times r}$, $G \in \mathbb{R}^{m \times r}$.

If n, m large, but $r \ll n, m$
$\rightsquigarrow$ X has a small numerical rank.
[Penzl 1999, Grasedyck 2004, Antoulas/Sorensen/Zhou 2002]

$$\operatorname{rank}(X, \tau) = f \ll \min(n, m)$$

singular values of 1600 × 900 example



$\rightsquigarrow$ Compute low-rank solution factors $Z \in \mathbb{R}^{n \times f}$, $Y \in \mathbb{R}^{m \times f}$, $D \in \mathbb{R}^{f \times f}$, such that $X \approx ZDY^T$ with $f \ll \min(n, m)$.

Lyapunov Equations

Find $X \in \mathbb{R}^{n \times n}$ solving

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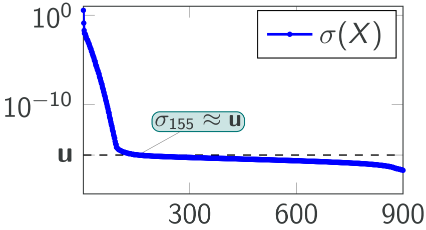

⇝ Compute low-rank solution factors $Z \in \mathbb{R}^{n \times f}$, $D \in \mathbb{R}^{f \times f}$, such that $X \approx ZDZ^T$ with $f \ll n$.

Consider $AX - XB + FG^T = 0$ with $\Lambda(A) \subset \mathbb{C}^-$ and $\Lambda(B) \subset \mathbb{C}^+$.

Definition

Recall: the matrix sign function of $M \in \mathbb{R}^{n \times n}$ with no purely imaginary eigenvalues is

$$\operatorname{sign}(M) = \operatorname{sign}\left(T \begin{bmatrix} J_- & 0 \\ 0 & J_+ \end{bmatrix} T^{-1} \right) = T \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix} T^{-1}$$

with $J_\pm$ containing all Jordan blocks of M corresponding to eigenvalues with positive/negative real parts.

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Observations

1. $\operatorname{sign}\left(\begin{bmatrix} A & FG^T \\ 0 & B \end{bmatrix}\right) = \begin{bmatrix} -I & 2X \\ 0 & I \end{bmatrix}$.
2. $\operatorname{sign}(M) = \lim_{k\to\infty} M_k$ with $M_{k+1} = \frac{1}{2}(M_k + M_k^{-1})$ if $M_0 = M$.

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Sign function iteration for solving Sylvester equations

$M_0 = \begin{bmatrix} A_0 & F_0 G_0^T \\ 0 & B_0 \end{bmatrix} = \begin{bmatrix} A & FG^T \\ 0 & B \end{bmatrix}$, and inversion formula for block-triangular matrices:

$$A_{k+1} \leftarrow \frac{1}{2}(A_k + A_k^{-1}), \qquad B_{k+1} \leftarrow \frac{1}{2}(B_k + B_k^{-1}),$$

$$F_{k+1}G_{k+1}^T \leftarrow \frac{1}{2}(F_k G_k^T + A_k^{-1} F_k G_k^T B_k^{-1}) = \frac{1}{2}[\,F_k,\ A_k^{-1}F_k\,][\,G_k,\ B_k^{-T}G_k]^T,$$

so that $F_k G_k^T \to 2X$.

Consider $AX - XB + FG^T = 0$ with $\Lambda(A) \subset \mathbb{C}^-$ and $\Lambda(B) \subset \mathbb{C}^+$.

Factored sign function iteration for Sylvester equations [B. 2004]

$$\begin{aligned} A_{k+1} &\leftarrow \frac{1}{2}(A_k + A_k^{-1}), & B_{k+1} &\leftarrow \frac{1}{2}(B_k + B_k^{-1}), \\ F_{k+1} &\leftarrow \frac{1}{\sqrt{2}}[\, F_k,\ A_k^{-1} F_k \,], & G_{k+1} &\leftarrow \frac{1}{\sqrt{2}}[\, G_k,\ B_k^{-T} G_k \,] \end{aligned}$$

Problem: number of columns in F_k, G_k doubles each iteration!

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Problem: number of columns in F_k, G_k doubles each iteration!

Cure: truncation operator

$$F_{k+1} \leftarrow \mathcal{T}_\varepsilon\left(\frac{1}{\sqrt{2}}[\,F_k,\ A_k^{-1}F_k\,]\right)$$

with, e.g., $\mathcal{T}_\varepsilon$ returning the scaled left singular vectors of the truncated SVD w.r.t. the numerical rank tolerance ε, similar for G_{k+1}.

Sylvester and Stein equations

Let $\alpha \neq \beta$ with $\alpha \notin \Lambda(B)$, $\beta \notin \Lambda(A)$, then

$$\underbrace{AX - XB = FG^T}_{\text{Sylvester equation}} \quad \Leftrightarrow \quad \underbrace{X = \mathcal{A} X \mathcal{B} + (\beta - \alpha)\mathcal{F}\mathcal{G}^H}_{\text{Stein equation}}$$

with the Cayley like transformations

$$\mathcal{A} := (A - \beta I_n)^{-1}(A - \alpha I_n), \qquad \mathcal{B} := (B - \alpha I_m)^{-1}(B - \beta I_m),$$
$$\mathcal{F} := (A - \beta I_n)^{-1} F, \qquad \mathcal{G} := (B - \alpha I_m)^{-H} G.$$

$\rightsquigarrow$ fix point iteration

$$X_k = \mathcal{A} X_{k-1} \mathcal{B} + (\beta - \alpha)\mathcal{F}\mathcal{G}^H$$

for $k \geq 1$, $X_0 \in \mathbb{R}^{n \times m}$.

Sylvester and Stein equations

Let $\alpha_\mathbf{k} \neq \beta_\mathbf{k}$ with $\alpha_\mathbf{k} \notin \Lambda(B)$, $\beta_\mathbf{k} \notin \Lambda(A)$, then

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with the Cayley like transformations

$$\mathcal{A}_\mathbf{k} := (A - \beta_\mathbf{k} I_n)^{-1}(A - \alpha_\mathbf{k} I_n), \qquad \mathcal{B}_\mathbf{k} := (B - \alpha_\mathbf{k} I_m)^{-1}(B - \beta_\mathbf{k} I_m),$$
$$\mathcal{F}_\mathbf{k} := (A - \beta_\mathbf{k} I_n)^{-1} F, \qquad \mathcal{G}_\mathbf{k} := (B - \alpha_\mathbf{k} I_m)^{-H} G.$$

$\rightsquigarrow$ **alternating directions implicit (ADI)** iteration

$$X_k = \mathcal{A}_\mathbf{k} X_{k-1} \mathcal{B}_\mathbf{k} + (\beta_\mathbf{k} - \alpha_\mathbf{k}) \mathcal{F}_\mathbf{k} \mathcal{G}_\mathbf{k}^H$$

for $k \geq 1$, $X_0 \in \mathbb{R}^{n \times m}$. [Wachspress 1988]

Sylvester ADI iteration [Wachspress 1988]

$$X_k = \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H,$$

$$\mathcal{A}_k := (A - \beta_k I_n)^{-1}(A - \alpha_k I_n), \quad \mathcal{B}_k := (B - \alpha_k I_m)^{-1}(B - \beta_k I_m),$$

$$\mathcal{F}_k := (A - \beta_k I_n)^{-1} F \in \mathbb{R}^{n\times r}, \quad \mathcal{G}_k := (B - \alpha_k I_m)^{-H} G \in \mathbb{C}^{m\times r}.$$

Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_1 = \mathcal{A}_1 X_0 \mathcal{B}_1 + (\beta_1 - \alpha_1)\mathcal{F}_1 \mathcal{G}_1^H$$

Sylvester ADI iteration [Wachspress 1988]

$$X_k = \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k) \mathcal{F}_k \mathcal{G}_k^H,$$
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Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_1 = (\beta_1 - \alpha_1)(A - \beta_1 I_n)^{-1} F G^T (B - \alpha_1 I_m)^{-1}$$
$$\Rightarrow V_1 := Z_1 = (A - \beta_1 I_n)^{-1} F \in \mathbb{R}^{n \times r}, \quad D_1 = (\beta_1 - \alpha_1) I_r \in \mathbb{R}^{r \times r},$$
$$W_1 := Y_1 = (B - \alpha_1 I_m)^{-H} G \in \mathbb{C}^{m \times r}.$$

Sylvester ADI iteration [Wachspress 1988]

$$X_k = \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H,$$

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Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_2 = \mathcal{A}_2 X_1 \mathcal{B}_2 + (\beta_2 - \alpha_2)\mathcal{F}_2 \mathcal{G}_2^H = \ldots =$$

$$V_2 = V_1 + (\beta_2 - \alpha_1)(A + \beta_2 I)^{-1} V_1 \in \mathbb{R}^{n \times r},$$

$$W_2 = W_1 + \overline{(\alpha_2 - \beta_1)}(B + \alpha_2 I)^{-H} W_1 \in \mathbb{R}^{m \times r},$$

$$Z_2 = [Z_1,\ V_2], \qquad D_2 = \operatorname{diag}(D_1, (\beta_2 - \alpha_2) I_r),$$

$$Y_2 = [Y_1,\ W_2].$$

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Algorithm [B. 2005, Li/Truhar 2008, B./Li/Truhar 2009]

Algorithm 2 Low-rank Sylvester ADI / factored ADI (fADI)

Input: Matrices defining $AX - XB = FG^T$ and shift parameters $\{\alpha_1, \ldots, \alpha_{k_{\max}}\}$, $\{\beta_1, \ldots, \beta_{k_{\max}}\}$.

Output: Z, D, Y such that $ZDY^H \approx X$.

$Z_1 = V_1 = (A - \beta_1 I_n)^{-1} F$.

$Y_1 = W_1 = (B - \alpha_1 I_m)^{-H} G$.

$D_1 = (\beta_1 - \alpha_1) I_r$

for $k = 2, \ldots, k_{\max}$ **do**

  $V_k = V_{k-1} + (\beta_k - \alpha_{k-1})(A - \beta_k I_n)^{-1} V_{k-1}$.

  $W_k = W_{k-1} + (\alpha_k - \beta_{k-1})(B - \alpha_k I_n)^{-H} W_{k-1}$.

  Update solution factors

  $Z_k = [Z_{k-1}, V_k]$, $Y_k = [Y_{k-1}, W_k]$, $D_k = \operatorname{diag}(D_{k-1}, (\beta_k - \alpha_k) I_r)$.

end for

Optimal Shifts

Solution of rational optimization problem

$$\min_{\substack{\alpha_j \in \mathbb{C} \\ \beta_j \in \mathbb{C}}} \max_{\substack{\lambda \in \Lambda(A) \\ \mu \in \Lambda(B)}} \prod_{j=1}^{k} \left| \frac{(\lambda - \alpha_j)(\mu - \beta_j)}{(\lambda - \beta_j)(\mu - \alpha_j)} \right|,$$

for which no analytic solution is known in general.

Optimal Shifts

Solution of rational optimization problem

$$\min_{\substack{\alpha_j \in \mathbb{C} \\ \beta_j \in \mathbb{C}}} \max_{\substack{\lambda \in \Lambda(A) \\ \mu \in \Lambda(B)}} \prod_{j=1}^{k} \left| \frac{(\lambda - \alpha_j)(\mu - \beta_j)}{(\lambda - \beta_j)(\mu - \alpha_j)} \right|,$$

for which no analytic solution is known in general.

Some shift generation approaches:

- generalized Bagby points, [LEVENBERG/REICHEL 1993]
- adaption of Penzl's cheap heuristic approach available [PENZL 1999, LI/TRUHAR 2008]
  $\rightsquigarrow$ approximate $\Lambda(A)$, $\Lambda(B)$ by small number of Ritz values w.r.t. A, A^{-1}, B, B^{-1} via Arnoldi,
- just taking these Ritz values alone also works well quite often.

Disadvantages of Low-Rank ADI as of 2012:

1. No efficient stopping criteria:
   - Difference in iterates $\rightsquigarrow$ norm of added columns/step: not reliable, stops often too late.
   - Residual is a full dense matrix, can not be calculated as such.
2. Requires complex arithmetic for real coefficients when complex shifts are used.
3. Expensive (only semi-automatic) set-up phase to precompute ADI shifts.

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None of these disadvantages exists as of today
$\Longrightarrow$ speed-ups old vs. new LR-ADI can be up to 20!

Projection-based methods for Lyapunov equations with $A + A^T < 0$:

1. Compute orthonormal basis $\mathrm{range}(Z)$, $Z \in \mathbb{R}^{n \times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n$, $\dim \mathcal{Z} = r$.
2. Set $\hat{A} := Z^T A Z$, $\hat{B} := Z^T B$.
3. Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^T + \hat{B}\hat{B}^T = 0$.
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Examples:

- Krylov subspace methods, i.e., for $m = 1$:

$$\mathcal{Z} = \mathcal{K}(A, B, r) = \mathrm{span}\{B, AB, A^2B, \ldots, A^{r-1}B\}$$

[Saad 1990, Jaimoukha/Kasenally 1994, Jbilou 2002–2008].

- Extended Krylov subspace method (EKSM) [Simoncini 2007],

$$\mathcal{Z} = \mathcal{K}(A, B, r) \cup \mathcal{K}(A^{-1}, B, r).$$

- Rational Krylov subspace methods (RKSM) [Druskin/Simoncini 2011].

- FEM discretization of a simple 3D ocean circulation model (barotropic, constant depth) $\rightsquigarrow$ stiffness matrix $-A$ with $n = 42,249$, choose artificial constant term $B = \texttt{rand(n,5)}$.

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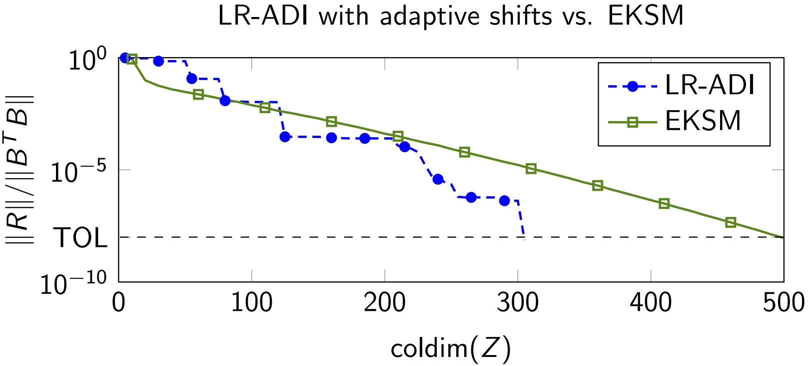
- **Convergence history:**



Numerical Performance

Example: an ocean circulation problem[Van Gijzen et al. 1998]

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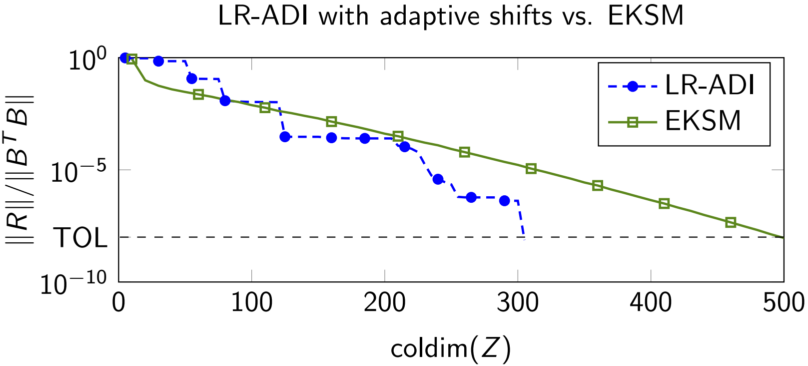

- CPU times: LR-ADI $\approx$ 110 sec, EKSM $\approx$ 135 sec.

- Numerical enhancements of low-rank ADI for large Sylvester/Lyapunov equations:
  1. low-rank residuals, reformulated implementation,
  2. compute real low-rank factors in the presence of complex shifts,
  3. self-generating shift strategies (quantification in progress).

For diffusion-convection-reaction example:
332.02 sec. down to **17.24 sec.** $\rightsquigarrow$ acceleration by factor almost **20**.

- Generalized version enables derivation of low-rank solvers for various generalized Sylvester equations.
- Ongoing work:
  - Apply LR-ADI in Newton methods for algebraic Riccati equations

$$\mathcal{D}(X) = AXA^T - EXE^T + GG^T + A^TXF(I_r + F^TXF)^{-1}F^TXA = 0.$$

- For nonlinear AREs see

P. Benner, P. Kürschner, J. Saak. *Low-rank Newton-ADI methods for large nonsymmetric algebraic Riccati equations.* J. Franklin Inst., 353(5):1147–1167, 2016.

Further Reading

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SIAM Journal on Control and Optimization 49(2):686–711, 2011.

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Numerical solution of large and sparse continuous time algebraic matrix Riccati and Lyapunov equations: a state of the art survey.
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