A new low-rank solver for algebraic Riccati equations based on the matrix sign function and principal pivot transforms

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joint work with Federico Poloni (Università di Pisa)

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Outline

Algebraic Riccati equation (ARE)

For $A, G = G^T, W = W^T \in \mathbb{R}^{n \times n}$ given and $X \in \mathbb{R}^{n \times n}$ unknown:

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- model reduction of (unstable) linear time-invariant (LTI) systems,
- linear-quadratic optimal control problems for LTI systems,
- H_∞-control, ...

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Typical situation in model reduction and control:

- G, W low-rank with $G, W \in \{BB^T, C^T C\}$, where $B \in \mathbb{R}^{n \times m}$, $m \ll n$, and $C \in \mathbb{R}^{p \times n}$, $p \ll n$.
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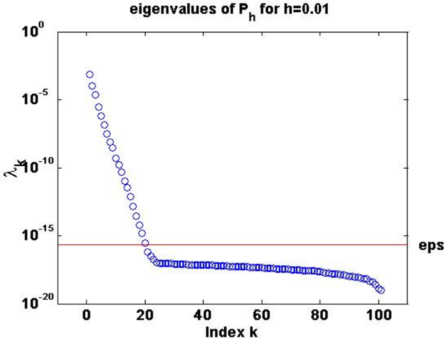
- **Want:** solution with $X = X^T \geq 0$ (and $\Lambda\,(A - GX) \subset \mathbb{C}^-$), notation: $X_\geq$.
- $n = 10^3 - 10^6$
  $\Longrightarrow$ X has $10^6 - 10^{12}$ unknowns
  $\Longrightarrow$ as X is dense in general, we face a storage problem!

Consider spectrum of ARE solution.

Example:

- Linear 1D heat equation with point control,
- $\Omega = [0, 1]$,
- FEM discretization using linear B-splines,
- $h = 1/100 \Longrightarrow n = 101$.



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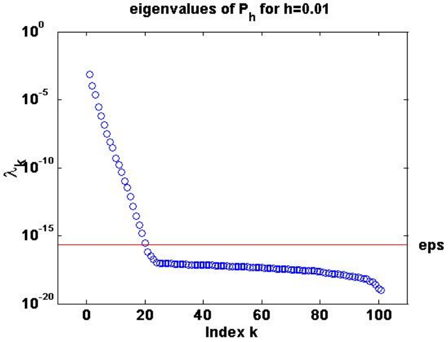

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Idea: $X = X^T \geq 0 \implies$

$$X = ZZ^T = \sum_{k=1}^{n} \lambda_k z_k z_k^T \approx \sum_{k=1}^{r} \lambda_k z_k z_k^T = \sum_{k=1}^{r} \left(\sqrt{\lambda_k} z_k\right) \left(\sqrt{\lambda_k} z_k\right)^T =: Z^{(r)}(Z^{(r)})^T.$$

$\implies$ **Goal:** compute $Z^{(r)} \in \mathbb{R}^{n \times r}$ directly w/o ever forming X!

$\exists$ many numerical methods to solve AREs.

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Definition

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

the matrix sign function is

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

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Lemma

Let $T \in \mathbb{R}^{n\times n}$ be nonsingular and Z as before, then

$$\operatorname{sign}\left(TZT^{-1}\right) = T \operatorname{sign}(Z)\, T^{-1}.$$

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Here: revisit the **matrix sign function method.**

Computation of $\operatorname{sign}(Z)$

$\operatorname{sign}(Z)$ is root of $I_n \Longrightarrow$ use Newton's method to compute it:

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

$\Longrightarrow \quad \operatorname{sign}(Z) = \lim_{j\to\infty} Z_j.$

$c_j > 0$ is scaling parameter for convergence acceleration and rounding error minimization, e.g.

$$c_j = \sqrt{\frac{\left\|Z_j^{-1}\right\|_F}{\|Z_j\|_F}},$$

based on "equilibrating" the norms of the two summands [Higham 1986].

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$$H \begin{bmatrix} I_n \\ -X_\geq \end{bmatrix} = \begin{bmatrix} I_n \\ -X_\geq \end{bmatrix} (A - GX_\geq),$$

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2. $\frac{1}{2}(I_{2n} + \operatorname{sign}(H))$ is a projector onto the H-invariant subspace corresponding to its left-half-plane eigenvalues

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$$\Longrightarrow \qquad (I_{2n} + \text{sign}(H)) \begin{bmatrix} I_n \\ -X_{\geq} \end{bmatrix} = 0.$$

3. Hence, $X_{\geq}$ is determined by overdetermined, but consistent linear system of equations once $\text{sign}(H)$ is known.

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1. Keep the off-diagonal blocks in H in low-rank form — this would save a significant amount of memory, i.e., working with A, B, C directly would reduce memory requirements by a factor of $\sim 3 - 4$.
2. Obtain $X_{\geq}$ in low-rank factored form directly.

Theorem (Kenney/Laub/Jonckheere 1989, B. 2019/22)

Let (A, B) be stabilizable, (A, C) be detectable, and define the Hamiltonian matrix

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Hence, $A - BB^TX_s$ is stable, the closed-loop Lyapunov equations

$$\begin{aligned} (A - BB^TX_\geq)P + P(A - BB^TX_\geq)^T + BB^T &= 0, \\ (A - BB^TX_\geq)^TQ + Q(A - BB^TX_\geq) + C^TC &= 0, \end{aligned}$$

have unique solutions $P = P^T \geq 0$, $Q = Q^T \geq 0$, resp., and it holds

$$\operatorname{sign}(H) = \begin{bmatrix} -I + 2PX_\geq & -2P \\ 2X_\geq PX_\geq - 2X_\geq & I - 2X_\geq P \end{bmatrix}.$$

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Hence, P (and by duality, Q) can be obtained from $\operatorname{sign}(H)$ directly, without solving the AREs at all, and in factored form if sign iterates preserve the off-diagonal low-rank structure!

Quasi-semidefinite Sign Function Iteration

Re-write the sign function iteration for $H = \begin{bmatrix} A & BB^T \\ C^TC & -A^T \end{bmatrix}$ in "symmetrized" form:

$$\frac{1}{2}\left(H + H^{-1}\right) = \frac{1}{2}\left(H + (J^TJH)^{-1}\right) = \frac{1}{2}\left(HJ^T + (JH)^{-1}\right)J =: \frac{1}{2}\left(\tilde{M} + M^{-1}\right)J,$$

where

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \qquad M = \begin{bmatrix} C^TC & -A^T \\ -A & -BB^T \end{bmatrix}, \qquad \tilde{M} = \begin{bmatrix} BB^T & -A \\ -A^T & -C^TC \end{bmatrix}.$$

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1. is numerically more robust than standard inversion of symmetric matrices,
2. allows to work directly with A, B, C without ever forming $2n \times 2n$-matrices,
3. yields a sign function iteration for AREs using A, B, C without ever forming $2n \times 2n$-matrices!

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Repeating this m times with pivots of size u_k, so that $u_0 + \cdots + u_{m-1} = n$, yields $M^{(m)} = -M^{-1}$, i.e., a **Gauß-Jordan-type inversion** procedure for symmetric matrices.

Inversion of Symmetric Matrices

Most software packages compute inverses of symmetric matrices M using LDL^T factroization with Bunch-Kaufman (diagonal, partial) or Bunch-Parlett (complete) pivoting, e.g., xSYTRI from LAPACK and the MATLAB function `inv` based on this. SQSD structure is usually ignored, but turns out to be beneficial!

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Theorem (Bunch–Parlett)

Let $LDL^T = \Pi M \Pi^T$ be the LDL^T factorization with Bunch–Parlett pivoting of a symmetric matrix M, with pivoting threshold $\tau = \frac{1+\sqrt{17}}{8} \approx 0.64$. Then,

$$\|D\|_{\max} \leq (2.57)^{n-1} \|M\|_{\max}, \quad \text{and} \quad \|L\|_{\max} \leq 2.78.$$

Here: a scalar pivot is chosen if $\max_{k=1,\ldots,n} |M[k,k]| \geq \tau \max_{i\neq j} |M[i,j]|$, if such k exists; otherwise maximum 2×2 pivot is chosen.

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Worst-case element growth can be slightly improved for SQSD matrices:

Theorem (B./Poloni 2019)

Let $LDL^T = \Pi M \Pi^T$ be the LDL^T factorization with Bunch–Parlett pivoting of a SQSD matrix M, with pivoting threshold $\tau = 1$. Then,

1. $\|D\|_{\max} \leq 2^{n-1} \|M\|_{\max}$, *and* $\|L\|_{\max} \leq 2$.
2. $\left\| |D| \left| D^{-1} \right| \right\|_{\max} \leq 2$, *and* $\left\| |D| \left| D^{-1} \right| \right\| \leq 3$.

Theorem (Backward stability of symmetric GJE)

Let $\hat{X}$ be the approximation of $X = -M^{-1}$ computed by the PPT-based symmetric Gauss–Jordan elimination algorithm. Then, each column $\hat{x}_j = \hat{X} e_j$ satisfies

$$-e_j = (M + \Delta_j)\hat{x}_j, \quad |\Delta_j| \leq |M| \left| L^{-T} \right| \left| L^T \right| \varepsilon_n,$$

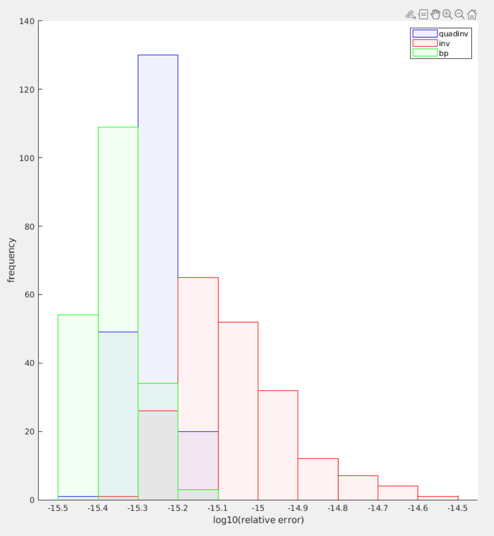
where $\varepsilon_n := \frac{cn\mathbf{u}}{1 - cn\mathbf{u}}$ with a constant c independent of n.

Inversion of 200 random 200×200 SQD matrices with

- MATLAB `inv`, based on DSYTRI from LAPACK
- Bunch-Parlett with complete pivoting,
- structured inversion using PPTs.

Inversion of 200 random 200×200 SQD matrices with

- MATLAB `inv`, based on DSYTRI from LAPACK
- Bunch-Parlett with complete pivoting,
- structured inversion using PPTs.



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Recall: $M_+ =: \frac{1}{2}\left(\tilde{M} + M^{-1}\right) J$ with $M, \tilde{M}$ SQSD.

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- Inversion can be implemented using A, B, C only using again PPT-variant applied to generator matrix

$$\mathfrak{G} = \begin{bmatrix} B & A \\ * & C \end{bmatrix},$$

i.e., compute $\mathfrak{X} = \begin{bmatrix} \hat{B} & \hat{A} \\ * & \hat{C} \end{bmatrix}$ representing M^{-1} using A, B, C only without ever forming M [Poloni/Strabić 2016]!

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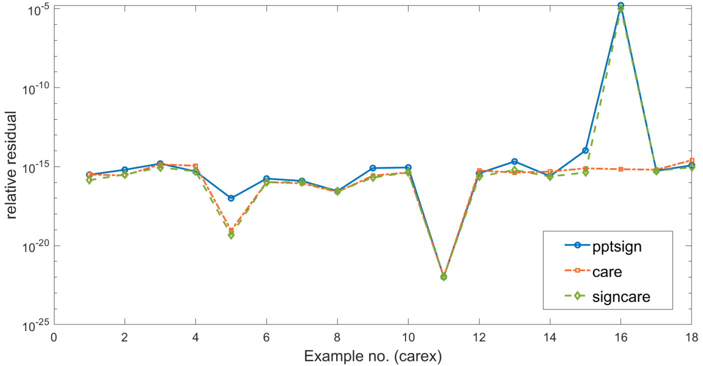
$\rightsquigarrow$ new version of sign function iteration working directly on generators!

Test the new sign function iteration for AREs based on PPTs (pptsign)

- vs. MATLAB function care (based on Schur vector method) and classical sign function method (signcare) from MORLab [B./Werner 2006–2023],
- using 18 examples from carex benchmark collection [B./Laub/Mehrmann 1995].

Measure accuracy by $\frac{\left\|\mathcal{R}(\tilde{X})\right\|_F}{\left\|C^TC\right\|_F + 2\|A\|_F\left\|\tilde{X}\right\|_F + \left\|BB^T\right\|_F\left\|\tilde{X}^2\right\|_F}$.



Conclusions

- Symmetric quasi-semidefinite matrices can be inverted using PPT-based Gauß-Jordan type elimination in a structure-preserving and numerically robust way.
- Sign function iteration for AREs can be reformulated in terms of SQSD matrix inversions and summations, allowing to work with generator matrices (A, B, C) only, without ever forming $2n \times 2n$ matrices.
- Leads to much lower storage requirements and potentially to faster algorithms (fewer flops).
- Application: cloed-loop balanced truncation without ever solving AREs.
- Future work: sophisticated implementation to really test performance.

P. Benner.
An alternative algorithm for unstable balanced truncation.
MATHMOD 2022 Discussion Contributions, ARGESIM Report 17, pp. 71–72, 2022.
DOI: 10.11128/arep.17.a17178

P. Benner, P. Ezzatti, E.S. Quintana-Ortí, A. Remón.
A factored variant of the Newton iteration for the solution of algebraic Riccati equations via the matrix sign function.
Numerical Algorithms, 66:363—377, 2014.

P. Benner, M. Köhler, and J. Saak.
Matrix equations, sparse solvers: M-M.E.S.S.-2.0.1 – philosophy, features and application for (parametric) model order reduction.
In Model Reduction of Complex Dynamical Systems, P. Benner, T. Breiten, H. Faßbender, M. Hinze, T. Stykel, and R. Zimmermann, eds., ISNM 171, Birkhäuser, Cham, pp. 369–392, 2021.

P. Benner and S. W. R. Werner.
MORLAB – A model order reduction framework in MATLAB and Octave.
In Mathematical Software – ICMS 2020, A. M. Bigatti, J. Carette, J. H. Davenport, M. Joswig, and T. de Wolff, eds., LNCS 12097, Springer International Publishing, Cham, pp. 432–441, 2020.

C. Kenney, A. J. Laub, and E. A. Jonckheere.
Positive and negative solutions of dual Riccati equations by matrix sign function iteration.
Systems Control Letters, 13:109–116, 1989.

F. Poloni and N. Strabić.
Principal pivot transforms of quasidefinite matrices and semidefinite Lagrangian subspaces.
Electronic Journal of Linear Algebra, 31:200–231, 2016.

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