Preconditioning Techniques for Multiterm Generalized Sylvester Equations

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Yannis Voet

Chair of Modeling and Numerical Simulation
EPFL

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Introduction

We consider solving generalized multiterm Sylvester equations

$$\sum_{k=1}^{r} B_k X A_k^T = E$$

where $A_k \in \mathbb{R}^{n\times n}$, $B_k \in \mathbb{R}^{m\times m}$ for all $k = 1, \ldots, r$ and $X, E \in \mathbb{R}^{m\times n}$.

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Now appear in an increasing number of applications:

- Finite difference (Palitta and Simoncini 2016; Hao and Simoncini 2021) and finite element (Ernst et al. 2009; Ullmann 2010; Mantzaflaris et al. 2017; Scholz et al. 2018) discretizations of (stochastic) PDEs [cf. Catherine Powell's talk at SIAM LA24]

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Includes as particular cases the famed (standard) Sylvester, Lyapunov and Stein equations.

Difficulties

Solution strategies critically depend on the number of terms r, the overall structure of the equation and properties of the coefficients.

$r = 1$:

$$B_1 X A_1^T = E$$

Trivial.

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$r = 2$:

$$B_1 X A_1^T + B_2 X A_2^T = E$$

Much more challenging:

- Direct solution techniques (Bartels and Stewart 1972; Gardiner et al. 1992).
- Block recursive splitting (Jonsson and Kågström 2002a; Jonsson and Kågström 2002b).
- Alternating Direction Implicit (ADI) (Wachspress 1988).
- Data-sparse methods (e.g. low-rank) (Massei et al. 2018; Palitta and Simoncini 2018; Grasedyck 2004; Kressner and Tobler 2010).
- Matrix oriented (truncated) CG/GMRES/... (Hochbruck and Starke 1995).

See e.g. Simoncini 2016; Benner and Saak 2013 for an overview.

Difficulties

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$r \geq 3$:

$$\sum_{k=1}^{r} B_k X A_k^T = E \tag{1}$$

- Low-rank methods (Benner and Breiten 2013; Kressner and Sirković 2015; Jarlebring et al. 2018).
- ADI (Benner and Saak 2013).
- Matrix oriented (truncated) CG/GMRES/... (Jbilou et al. 1999; Bouhamidi and Jbilou 2008).

Notes:

- No general direct solution method for $r \geq 3$ with complexity $O(n^3 + m^3)$.
- Projection type techniques require solving a small size version of (1).

Kronecker form

Define the linear operator $\mathcal{M}\colon \mathbb{R}^{m\times n} \to \mathbb{R}^{m\times n}$ and its Kronecker representation $M \in \mathbb{R}^{mn\times mn}$ as

$$\mathcal{M}(X) = \sum_{k=1}^{r} B_k X A_k^T, \quad M = \sum_{k=1}^{r} A_k \otimes B_k.$$

Exploit the equivalence

$$\mathcal{M}(X) = Y \iff M\mathbf{x} = \mathbf{y}$$

with $\mathbf{x} = \mathrm{vec}(X)$, $\mathbf{y} = \mathrm{vec}(Y)$.

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👎 Limited to small or medium size equations ($m, n < 10^4$).

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Equivalent to the (matrix) low-rank approximation problem

$$\min \|\mathcal{R}(M) - \operatorname{vec}(Y) \operatorname{vec}(Z)^T\|_F$$

where $\mathcal{R} \colon \mathbb{R}^{nm \times nm} \to \mathbb{R}^{n^2 \times m^2}$ is a rearrangement operator.

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Algorithm:

1. Compute the "SVD representation" of M via the SVD of $\mathcal{R}(M)$

$$\mathcal{R}(M) = \sum_{k=1}^{r} \sigma_k \mathbf{u}_k \mathbf{v}_k^T \iff M = \sum_{k=1}^{r} \sigma_k (U_k \otimes V_k).$$

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2. Retain the leading $q \leq 2$ terms and use it as preconditioner

$$P = \sum_{k=1}^{q} \sigma_k (U_k \otimes V_k).$$

Theoretical results

- For $q = 1$, P is block-banded, nonnegative and positive definite if M is (Van Loan and Pitsianis 1993, Theorems 5.1, 5.3 and 5.8).

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Theorem

If $M, P \in \mathbb{R}^{n \times n}$ are symmetric positive definite

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(1 - \frac{1}{\lambda_i(M,P)}\right)^2} \leq \kappa(M)\sqrt{\sum_{k=q+1}^{r}\left(\frac{\sigma_k}{\sigma_1}\right)^2}.$$

$\rightarrow$ Effective preconditioner if $\mathcal{R}(M)$ features a fast singular value decay.

Kronecker approximate inverse

Find factor matrices $C \in \mathbb{R}^{n\times n}$ and $D \in \mathbb{R}^{m\times m}$ such that $C \otimes D \approx \left(\sum_{k=1}^{r} A_k \otimes B_k\right)^{-1}$.

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Use the reshaping that transforms

$$M = \begin{pmatrix} M_{11} & \dots & M_{1n} \\ \vdots & \ddots & \vdots \\ M_{n1} & \dots & M_{nn} \end{pmatrix} \quad \text{to} \quad \tilde{M} = \begin{pmatrix} M_{11} \\ M_{21} \\ \vdots \\ M_{nn} \end{pmatrix}$$

$\rightarrow$ Alternately solve a sequence of least squares problems for reshaped quantities

$$\min_{D} \|\tilde{I} - \mathcal{B} D\|_F \quad \text{and} \quad \min_{C} \|\hat{I} - \mathcal{A} C\|_F$$

$$\begin{aligned} \mathcal{B} &= (U \otimes I_m)B, & U &= [\mathrm{vec}(A_1 C), \dots, \mathrm{vec}(A_r C)], & B &= [B_1; B_2; \dots; B_r], \\ \mathcal{A} &= (V \otimes I_n)A, & V &= [\mathrm{vec}(B_1 D), \dots, \mathrm{vec}(B_r D)], & A &= [A_1; A_2; \dots; A_r]. \end{aligned}$$

Algorithm (via normal equations)

Input: Initial guess $C \in \mathbb{R}^{n \times n}$, tolerance $\epsilon > 0$ and number of iterations $N \in \mathbb{N}$
Output: C and D such that $C \otimes D \approx \left(\sum_{k=1}^{r} A_k \otimes B_k\right)^{-1}$

1: Set $r = \infty$, $j = 0$ ▷ Initialization
2: **while** $\sqrt{r} > \epsilon$ **and** $j \leq N$ **do**
▷ Optimizing for D
3: Compute $\beta_{kl} = \langle A_k^T A_l, CC^T \rangle_F$ for $k, l = 1, \dots, r$ ▷ $O(rn^3 + r^2 n^2)$
4: Compute $\delta_k = \langle A_k^T, C \rangle_F$ for $k = 1, \dots, r$ ▷ $O(rn^2)$
5: Form $\mathcal{B}^T \mathcal{B} = \sum_{k,l=1}^{r} \beta_{kl} B_k^T B_l$ ▷ $O(rm^3 + r^2 m^2)$
6: Form $\mathcal{B}^T \tilde{I} = \sum_{k=1}^{r} \delta_k B_k^T$ ▷ $O(rm^2)$
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13: Update β_{kl} and δ_k following lines 3 and 4, respectively ▷ Residual
14: Compute $r = nm - 2\sum_{k=1}^{r} \gamma_k \delta_k + \sum_{k,l=1}^{r} \alpha_{kl} \beta_{kl}$ ▷ $O(r^2)$
15: Update $j = j + 1$
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14: Compute $r = nm - 2\sum_{k=1}^{r} \gamma_k \delta_k + \sum_{k,l=1}^{r} \alpha_{kl} \beta_{kl}$ ▷ $O(r^2)$
15: Update $j = j + 1$
16: **end while**

Algorithm: ALS for Kronecker rank 1 approximate inverse

Algorithm (via normal equations)

Input: Initial guess $C \in \mathbb{R}^{n \times n}$, tolerance $\epsilon > 0$ and number of iterations $N \in \mathbb{N}$
Output: C and D such that $C \otimes D \approx \left(\sum_{k=1}^{r} A_k \otimes B_k\right)^{-1}$

1: Set $r = \infty$, $j = 0$ $\triangleright$ Initialization
2: **while** $\sqrt{r} > \epsilon$ **and** $j \leq N$ **do**
$\triangleright$ Optimizing for D
3: Compute $\beta_{kl} = \langle A_k^T A_l, CC^T \rangle_F$ for $k, l = 1, \ldots, r$ $\triangleright$ $O(rn^3 + r^2n^2)$
4: Compute $\delta_k = \langle A_k^T, C \rangle_F$ for $k = 1, \ldots, r$ $\triangleright$ $O(rn^2)$
5: Form $\mathcal{B}^T\mathcal{B} = \sum_{k,l=1}^{r} \beta_{kl} B_k^T B_l$ $\triangleright$ $O(rm^3 + r^2m^2)$
6: Form $\mathcal{B}^T\tilde{I} = \sum_{k=1}^{r} \delta_k B_k^T$ $\triangleright$ $O(rm^2)$
7: Solve $\mathcal{B}^T\mathcal{B}D = \mathcal{B}^T\tilde{I}$ $\triangleright$ $O(m^3)$
$\triangleright$ Optimizing for C
8: Compute $\alpha_{kl} = \langle B_k^T B_l, DD^T \rangle_F$ for $k, l = 1, \ldots, r$ $\triangleright$ $O(rm^3 + r^2m^2)$
9: Compute $\gamma_k = \langle B_k^T, D \rangle_F$ for $k = 1, \ldots, r$ $\triangleright$ $O(rm^2)$
10: Form $\mathcal{A}^T\mathcal{A} = \sum_{k,l=1}^{r} \alpha_{kl} A_k^T A_l$ $\triangleright$ $O(rn^3 + r^2n^2)$
11: Form $\mathcal{A}^T\tilde{I} = \sum_{k=1}^{r} \gamma_k A_k^T$ $\triangleright$ $O(rn^2)$
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- The residual directly controls the clustering of the eigenvalues of the preconditioned operator (Grote and Huckle 1997, Theorem 3.2). For $M, P \in \mathbb{R}^{n\times n}$

$$\sum_{i=1}^{n} |1-\lambda_i(MP)|^2 \leq \|I - MP\|_F^2.$$

Sparse Kronecker approximate inverse

Define sets of sparse matrices $\mathcal{S}_C \subset \mathbb{R}^{n\times n}$ and $\mathcal{S}_D \subset \mathbb{R}^{m\times m}$ with prescribed sparsity (based e.g. on powers of $\sum_{k=1}^r A_k$ and $\sum_{k=1}^r B_k$ or some variation) (Huckle 1999).

Solve alternately

$$\min_{D\in\mathcal{S}_D} \|\tilde{I} - \mathcal{B}D\|_F, \quad \text{and} \quad \min_{C\in\mathcal{S}_C} \|\hat{I} - \mathcal{A}C\|_F.$$

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If X is sparse, $\mathcal{P}(X)$ retains some sparsity. Let β_M denote the bandwidth of a matrix M.

Lemma

The Bi-CGSTAB method applied to $\mathcal{M}(X) = Y$ and preconditioned with $\mathcal{P}$ with starting matrix $X_0 = 0$ produces iterates X_j (for a full iteration $j \geq 1$) with bandwidth

$$\beta_{X_j} \leq (2j-1)(\beta_{\mathcal{M}} + \beta_{\mathcal{P}}) + \beta_{\mathcal{P}} + \beta_E$$

where $\beta_{\mathcal{M}} = \max_k\{\beta_{A_k} + \beta_{B_k}\}$ and $\beta_{\mathcal{P}} = \max_s\{\beta_{C_s} + \beta_{D_s}\}$.

RC circuit simulation

Lyapunov-plus-positive equation (Benner and Breiten 2013):

$$AX + XA^T + NXN^T = E, \tag{2}$$

with $m = n = 930$.

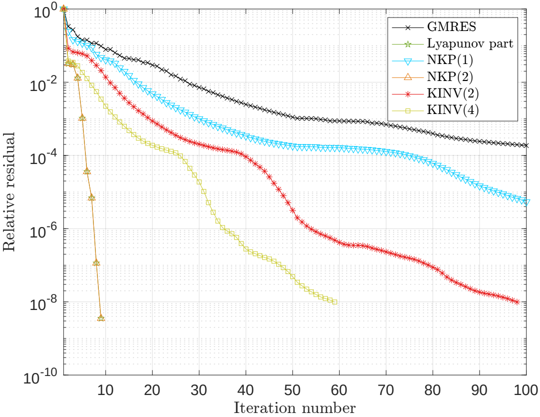


Figure: Convergence history for solving (2) using the (right-preconditioned) GMRES method. The non-preconditioned method converged after 630 iterations.

RC circuit simulation

Timings:

Preconditioner	Setup	GMRES
None	–	26.0 (630)
Lyapunov	–/6.0	12.2 (8)
NKP(1)	0.06/0.02	15.0 (203)
NKP(2)	0.06/5.9	12.2 (8)
KINV(2)	1.4	5.8 (97)
KINV(4)	2.4	5.2 (58)

Table: Timing (in seconds). When writing x/y, x represents the time for computing the SVD representation of the operator and y is the time for computing matrix factorizations (e.g. QZ or LU). The total number of iterations is shown in parenthesis.

Convection-diffusion equation

Consider the PDE (Palitta and Simoncini 2016)

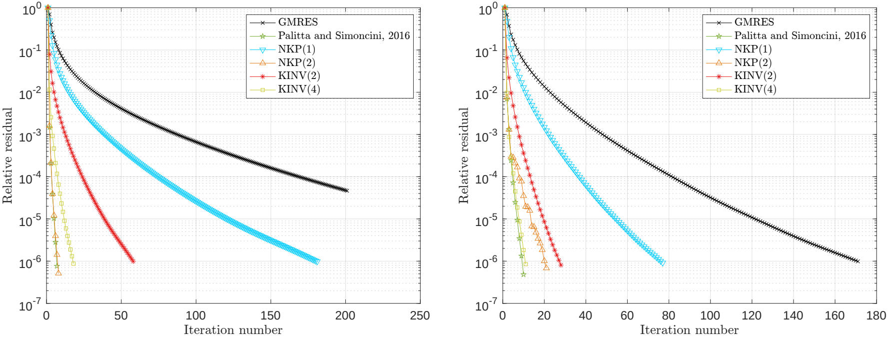
$$-\epsilon \Delta u + \mathbf{w} \cdot \nabla u = f \quad \text{on } \Omega = (0,1)^2.$$

Set suitable boundary conditions, $f = 0$ and

$$\mathbf{w} = \begin{pmatrix} y(1-(2x+1)^2) \\ -2(2x+1)(1-y^2) \end{pmatrix}.$$

Finite difference discretization on the grid $\{x_i\}_{i=1}^n \times \{y_j\}_{j=1}^n$ with $n = 1000$

$$TX + XT^T + (\Phi_1 B) X \Psi_1 + \Phi_2 X (B^T \Psi_2) = F \tag{3}$$



(a) $\epsilon = 1/10$

(b) $\epsilon = 1/30$

Convection-diffusion equation

Timings:

Preconditioner	Setup	$\epsilon = 1/10$	$\epsilon = 1/20$	$\epsilon = 1/30$
None	$-$	103.9 (200*)	105.1 (200*)	73.25 (170)
Palitta and Simoncini	$-$/10.3	10.8 (6)	14.2 (8)	24.4 (9)
NKP(1)	0.04/0.01	94.9 (180)	28.9 (104)	13.8 (76)
NKP(2)	0.04/8.95	13.4 (7)	20.7 (12)	51.1 (20)
KINV(2)	1.04	9.38 (57)	4.41 (35)	2.95 (27)
KINV(4)	1.86	2.04 (17)	1.40 (12)	1.17 (10)

Table: Timing (in seconds). When writing x/y, x represents the time for computing the SVD representation of the operator and y is the time for computing matrix factorizations (e.g. QZ or LU). The total number of iterations is shown in parenthesis, where $*$ indicates that the method did not converge within the maximum number of iterations.

Conclusions

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