Deflation techniques for two classes of structured linear systems

Kui Du

kuidu@xmu.edu.cn

School of Mathematical Sciences, Xiamen University

https://kuidu.github.io

joint work with Jia-Jun Fan and Fang Wang

Frontier Forum on Numerical Algebra
Suzhou, November 28–30, 2025

Outline

1. Linear systems, Krylov subspace methods, and deflation
2. Nonsymmetric positive definite linear systems
3. Symmetric quasi-definite linear systems
4. Summary

Linear systems, Krylov subspace methods, and deflation

- Linear systems of equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \qquad \mathbf{A} \in \mathbb{R}^{m \times m}, \qquad \mathbf{b} \in \mathbb{R}^{m}$$

- Krylov subspace methods

  CG, MINRES; GMRES, CMRH, Bi-CG, QMR, Bi-CGSTAB ...

- Acceleration techniques

  preconditioning, randomization, inexact or mixed-precision, inner-product free (orthogonalization-free), deflation ...

- When solving linear systems, deflation refers to reducing the influence of some eigenvalues that tend to slow convergence. Deflation can be implemented

  (1) by adding approximate eigenvectors to a subspace, or

  (2) by building a preconditioner from eigenvectors.

Some solvers incorporating augmentation-based deflation

- Nonsymmetric linear systems: Arnoldi + augmentation + restart
  FOM-IR, GMRES-IR (Morgan, SIMAX, 2000), FOM-DR, GMRES-DR (Morgan, SISC, 2002)

$$\mathbf{A}\mathbf{V}_m^{(i)} = \mathbf{V}_{m+1}^{(i)}\mathbf{H}_{m+1,m}^{(i)}, \quad i = 1, 2, \ldots$$

- Symmetric linear systems: Lanczos + augmentation + restart
  Lanczos-DR, MINRES-DR (Abdel-Rehim et al., SISC, 2010)

$$\mathbf{A}\mathbf{V}_m^{(i)} = \mathbf{V}_{m+1}^{(i)}\mathbf{T}_{m+1,m}^{(i)}, \quad i = 1, 2, \ldots$$

- Symmetric saddle point linear systems: Golub–Kahan + augmentation + restart
  Augmented LSQR (Baglama, Reichel, and Richmond, NA, 2013)
  Augmented CRAIG (Dumitrasc, Kruse, and Rüde, SIMAX, 2024)

$$\mathbf{A}\mathbf{V}_m^{(i)} = \mathbf{U}_{m+1}^{(i)}\mathbf{B}_{m+1,m}^{(i)}, \quad \mathbf{A}^\top\mathbf{U}_{m+1}^{(i)} = \mathbf{V}_{m+1}^{(i)}(\mathbf{B}_{m+1}^{(i)})^\top, \quad i = 1, 2, \ldots$$

Nonsymmetric positive definite linear systems

- The symmetric and skew-symmetric splitting

  $$\mathbf{A} = \mathbf{H} + \mathbf{S}, \quad \mathbf{H} := \frac{1}{2}(\mathbf{A} + \mathbf{A}^\top), \quad \mathbf{S} := \frac{1}{2}(\mathbf{A} - \mathbf{A}^\top).$$

  Assume that the symmetric part $\mathbf{H}$ of $\mathbf{A}$ is SPD.

- Stationary iterative methods

  HSS (Bai, Golub, and Ng, SIMAX, 2003) ...

- Krylov subspace methods based on the skew-symmetric Lanczos process

  CGW (Concus and Golub, 1976, Widlund, 1978) : Galerkin condition

  Rapoport's method (Rapoport, 1978): MR condition

Nonsymmetric positive definite linear systems

- Skew-symmetric Lanczos

$$\mathbf{S}\mathbf{U}_m = \mathbf{H}\mathbf{U}_{m+1}\mathbf{T}_{m+1,m}, \quad \mathbf{T}_{m+1,m} = \begin{bmatrix} 0 & -\gamma_2 & & \\ \gamma_2 & 0 & \ddots & \\ & \ddots & \ddots & -\gamma_m \\ & & \gamma_m & 0 \\ & & & \gamma_{m+1} \end{bmatrix} = \begin{bmatrix} \mathbf{T}_m \\ \gamma_{m+1}\mathbf{e}_m^\top \end{bmatrix}.$$

- Note that $\lambda(\mathbf{H}^{-1}\mathbf{S}) = \{\pm\sigma_1 \mathrm{i}, \pm\sigma_2 \mathrm{i}, \ldots, \pm\sigma_{r/2}\mathrm{i}, 0\}$ with $r = \operatorname{rank}(\mathbf{H}^{-1}\mathbf{S})$ and $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{r/2} > 0$.

  CGW convergence: $\dfrac{\|\mathbf{x}_{2j} - \mathbf{A}^{-1}\mathbf{b}\|_{\mathbf{H}}}{\|\mathbf{x}_0 - \mathbf{A}^{-1}\mathbf{b}\|_{\mathbf{H}}} \leq 2\left(\dfrac{\sqrt{1+\sigma_1^2}-1}{\sqrt{1+\sigma_1^2}+1}\right)^j$

  Rapoport convergence: $\dfrac{\|\mathbf{b} - \mathbf{A}\mathbf{x}_j\|_{\mathbf{H}^{-1}}}{\|\mathbf{b} - \mathbf{A}\mathbf{x}_0\|_{\mathbf{H}^{-1}}} \leq 2\left(\dfrac{\sigma_1}{\sqrt{1+\sigma_1^2}+1}\right)^j$

Skew-symmetric Lanczos with deflated restarting

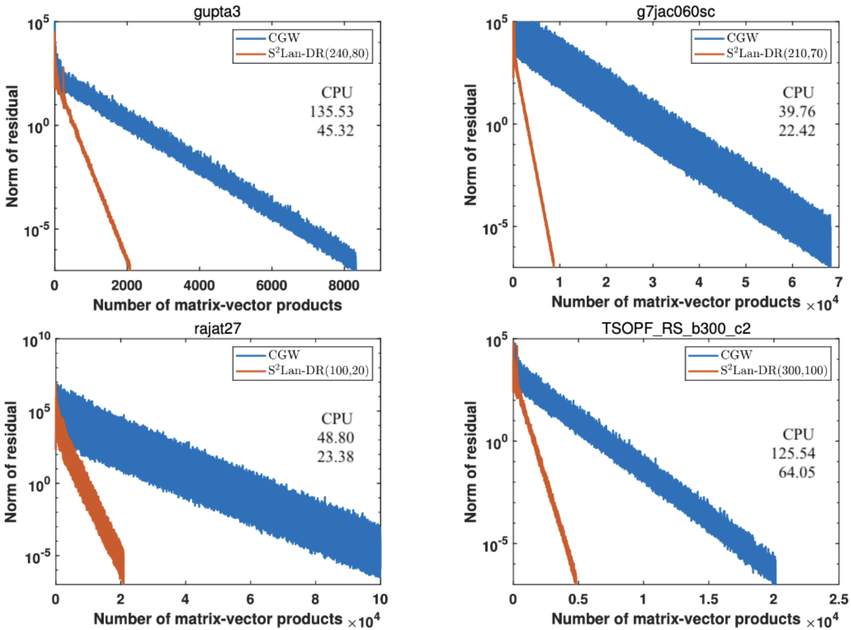
- $\mathsf{S^2Lan\text{-}DR}(m, 2k)$

$$\mathbf{S}\mathbf{U}_m^{(i)} = \mathbf{H}\mathbf{U}_{m+1}^{(i)}\mathbf{T}_{m+1,m}^{(i)}$$

For example, $m = 8$, $k = 2$, $i = 2, 3, \ldots,$

$$\mathbf{T}_{m+1,m}^{(i)} = \begin{bmatrix} 0 & \times & & & \times & & & \\ \times & 0 & & & \times & & & \\ & & 0 & \times & \times & & & \\ & & \times & 0 & \times & & & \\ \times & \times & \times & \times & 0 & \times & & \\ & & & & \times & 0 & \times & \\ & & & & & \times & 0 & \times \\ & & & & & & \times & 0 \\ & & & & & & & \times \end{bmatrix}, \quad \mathbf{T}_m^{(i)} = -(\mathbf{T}_m^{(i)})^\top.$$

CGW vs. S^2Lan-DR$(m, 2k)$



Rapoport with deflated restarting

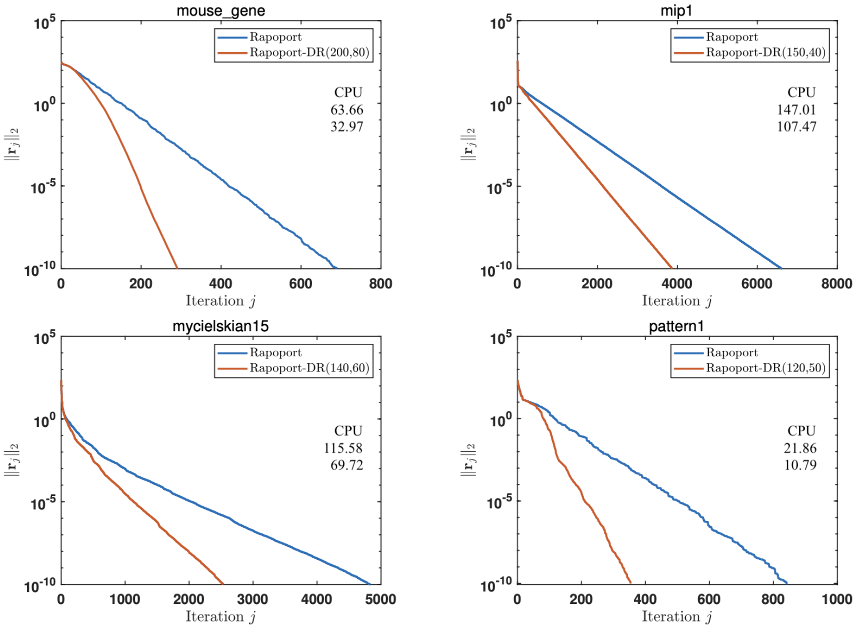
- Rapoport-DR$(m, 2k)$

$$\mathbf{S}\mathbf{U}_m^{(i)} = \mathbf{H}\mathbf{U}_{m+1}^{(i)}\mathbf{T}_{m+1,m}^{(i)}$$

For example, $m = 8$, $k = 2$, $i = 2, 3, \ldots,$

$$\mathbf{T}_{m+1,m}^{(i)} = \begin{bmatrix} 0 & \times & \times & \times & \times & & & \\ \times & 0 & \times & \times & \times & & & \\ \times & \times & 0 & \times & \times & & & \\ \times & \times & \times & 0 & \times & & & \\ \times & \times & \times & \times & 0 & \times & & \\ & & & & \times & 0 & \times & \\ & & & & & \times & 0 & \times \\ & & & & & & \times & 0 \\ & & & & & & & \times \end{bmatrix}, \quad \mathbf{T}_m^{(i)} = -(\mathbf{T}_m^{(i)})^\top.$$

Rapoport vs. Rapoport-DR($m, 2k$)



Symmetric quasi-definite linear systems

- $\mathbf{M} \in \mathbb{R}^{m \times m}$ and $\mathbf{N} \in \mathbb{R}^{n \times n}$ are SPD, $\mathbf{A} \in \mathbb{R}^{m \times n}$ is nonzero, $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{c} \in \mathbb{R}^n$:

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}, \quad \mathbf{H} = \begin{bmatrix} \mathbf{M} & \\ & \mathbf{N} \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix}.$$

- Symmetric, indefinite, nonsingular
- Monolithic methods: solving the system as a whole, for example, SYMMLQ, MINRES

  Segregated methods: tailored specifically to the block structure, for example,

  TriCG: generalized Saunders–Simon–Yip tridiagonalization + Galerkin condition, mathematically equivalent to preconditioned block-CG

  TriMR: generalized Saunders–Simon–Yip tridiagonalization + MR conditon, mathematically equivalent to preconditioned block-MINRES

  (Montoison and Orban, SISC, 2021)

The generalized SSY tridiagonalization

- Let $\beta_1 \mathbf{M}\mathbf{u}_1 = \mathbf{b}$ and $\gamma_1 \mathbf{N}\mathbf{v}_1 = \mathbf{c}$. After j steps of gSSY, we have

$$\mathbf{A}\mathbf{V}_j = \mathbf{M}\mathbf{U}_{j+1}\mathbf{T}_{j+1,j}, \quad \mathbf{A}^\top \mathbf{U}_j = \mathbf{N}\mathbf{V}_{j+1}\mathbf{T}_{j,j+1}^\top,$$

$$\mathbf{U}_{j+1}^\top \mathbf{M}\mathbf{U}_{j+1} = \mathbf{V}_{j+1}^\top \mathbf{N}\mathbf{V}_{j+1} = \mathbf{I}_{j+1}.$$

with

$$\mathbf{T}_{j+1,j} = \begin{bmatrix} \alpha_1 & \gamma_2 & & \\ \beta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \gamma_j \\ & & \beta_j & \alpha_j \\ & & & \beta_{j+1} \end{bmatrix} = \begin{bmatrix} \mathbf{T}_j \\ \beta_{j+1}\mathbf{e}_j^\top \end{bmatrix}.$$

M. A. Saunders, H. D. Simon, and E. L. Yip. *Two conjugate-gradient-type methods for unsymmetric linear equations.* SINUM, Vol. 25, Iss. 4 (1988)

TriCG

- Assume that no breakdowns occur for the first j steps, i.e., $\mathbf{U}_j$, $\mathbf{V}_j$, and $\mathbf{T}_j$ are well defined. The jth TriCG iterate is

$$\begin{bmatrix} \mathbf{x}_j \\ \mathbf{y}_j \end{bmatrix} = \begin{bmatrix} \mathbf{U}_j & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_j \end{bmatrix} \begin{bmatrix} \mathbf{I}_j & \mathbf{T}_j \\ \mathbf{T}_j^\top & -\mathbf{I}_j \end{bmatrix}^{-1} \begin{bmatrix} \beta_1 \mathbf{e}_1 \\ \gamma_1 \mathbf{e}_1 \end{bmatrix},$$

  which satisfies the Galerkin condition

$$\begin{bmatrix} \mathbf{U}_j & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_j \end{bmatrix}^\top \left(\begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix} - \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x}_j \\ \mathbf{y}_j \end{bmatrix} \right) = \mathbf{0}.$$

- Equivalent to preconditioned block-CG:

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x}^1 & \mathbf{x}^2 \\ \mathbf{y}^1 & \mathbf{y}^2 \end{bmatrix} = \begin{bmatrix} \mathbf{b} & \mathbf{0} \\ \mathbf{0} & \mathbf{c} \end{bmatrix}.$$

A. Montoison and D. Orban. *TriCG and TriMR: Two iterative methods for symmetric quasi-definite systems.* SISC, Vol. 43, Iss. 4 (2021)

Elliptic singular value decomposition (ESVD)

- Given SPD $\mathbf{M}$ and $\mathbf{N}$, ESVD of $\mathbf{A}$ is

$$\mathbf{A} = \mathbf{M}\mathbf{P}\mathbf{\Sigma}\mathbf{Q}^\top\mathbf{N},$$

where $\mathbf{\Sigma} = \mathrm{diag}(\sigma_1, \dots, \sigma_p)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, $p = \min(m, n)$, and $\mathbf{P}$ and $\mathbf{Q}$ satisfy

$$\mathbf{P}^\top\mathbf{M}\mathbf{P} = \mathbf{I}_m, \quad \mathbf{Q}^\top\mathbf{N}\mathbf{Q} = \mathbf{I}_n.$$

- Eigenvalues of a two-sided preconditioned matrix (let $r = \mathrm{rank}(\mathbf{A})$):

$$\lambda\left(\mathbf{H}^{-\frac{1}{2}}\mathbf{K}\mathbf{H}^{-\frac{1}{2}}\right) = \begin{cases} \pm\sqrt{\sigma_i^2 + 1}, & i = 1, \dots, r, \\ 1, & (m - r) \text{ times}, \\ -1, & (n - r) \text{ times}. \end{cases}$$

M. Arioli. *Generalized Golub–Kahan bidiagonalization and stopping criteria*. SIMAX, Vol. 34, Iss. 2 (2013)

A gSSY process with deflated restarting

- gSSY-DR(p,k):

$$\begin{aligned} \mathbf{A}\mathbf{V}_p^{(i)} &= \mathbf{M}\mathbf{U}_p^{(i)}\mathbf{T}_p^{(i)} + \beta_{p+1}^{(i)}\mathbf{M}\mathbf{u}_{p+1}^{(i)}\mathbf{e}_p^{\top}, \\ \mathbf{A}^{\top}\mathbf{U}_p^{(i)} &= \mathbf{N}\mathbf{V}_p^{(i)}(\mathbf{T}_p^{(i)})^{\top} + \gamma_{p+1}^{(i)}\mathbf{N}\mathbf{v}_{p+1}^{(i)}\mathbf{e}_p^{\top}. \end{aligned}$$

For $i = 2, 3, \dots,$

$$\mathbf{T}_p^{(i)} = \begin{bmatrix} \alpha_1^{(i)} & & & \gamma_2^{(i)} & & & \\ & \ddots & & \vdots & & & \\ & & \ddots & \gamma_{k+1}^{(i)} & & & \\ \beta_2^{(i)} & \dots & \beta_{k+1}^{(i)} & \alpha_{k+1}^{(i)} & \gamma_{k+2}^{(i)} & & \\ & & & \beta_{k+2}^{(i)} & \alpha_{k+2}^{(i)} & \ddots & \\ & & & & \ddots & \ddots & \gamma_p^{(i)} \\ & & & & & \beta_p^{(i)} & \alpha_p^{(i)} \end{bmatrix}.$$

TriCG with deflated restarting

- The recurrences in the first cycle are the same as that of TriCG. Now consider cycle $i \geq 2$. The jth $(k+1 \leq j \leq p)$ TriCG-DR(p,k) iterate is

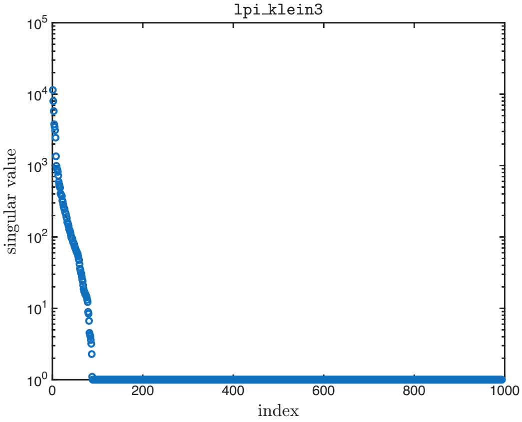
$$\begin{bmatrix} \mathbf{x}_j^{(i)} \\ \mathbf{y}_j^{(i)} \end{bmatrix} = \begin{bmatrix} \mathbf{U}_j^{(i)} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_j^{(i)} \end{bmatrix} \begin{bmatrix} \mathbf{I}_j & \mathbf{T}_j^{(i)} \\ (\mathbf{T}_j^{(i)})^\top & -\mathbf{I}_j \end{bmatrix}^{-1} \begin{bmatrix} \beta_1^{(i)} \mathbf{e}_{k+1} \\ \gamma_1^{(i)} \mathbf{e}_{k+1} \end{bmatrix},$$

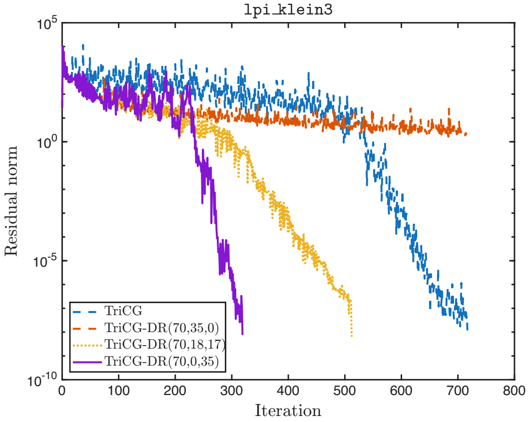
which satisfies the Galerkin condition

$$\begin{bmatrix} \mathbf{U}_j^{(i)} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_j^{(i)} \end{bmatrix}^\top \left(\begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix} - \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x}_j^{(i)} \\ \mathbf{y}_j^{(i)} \end{bmatrix} \right) = \mathbf{0}.$$

- Using an LDL$^\top$ decomposition and the same strategy in TriCG, short recurrences can be obtained to compute $\mathbf{x}_j^{(i)}$ and $\mathbf{y}_j^{(i)}$ for $k+1 \leq j \leq p$.

TriCG vs. TriCG-DR





Summary

- We have developed deflation techniques for nonsymmetric positive definite linear systems and symmetric quasi-definite linear systems.
- We have proposed S^2Lan-DR and Rapopart-DR for solving nonsymmetric positive definite linear systems, and TriCG-DR for solving symmetric quasi-definite linear systems. The new methods have faster convergence and demonstrate a significant advantage in computational time.
- S^2Lan-DR and gSSY-DR can be used to compute partial spectral information. And the computed spectral information can be used to help solve linear systems with sequential multiple right-hand sides.

Our recent related work

- Kui Du, Jia-Jun Fan, Xiao-Hui Sun, Fang Wang, and Ya-Lan Zhang
  On Krylov subspace methods for skew-symmetric and shifted skew-symmetric linear systems, Advances in Computational Mathematics (2024) 50:78
- Kui Du, Jia-Jun Fan, and Fang Wang
  On deflated CGW methods for solving nonsymmetric positive definite linear systems, Calcolo (2025) 62:22.
- Kui Du, Jia-Jun Fan, and Ya-Lan Zhang
  Improved TriCG and TriMR methods for symmetric quasi-definite linear systems
  Numerical Linear Algebra with Applications, 2025, 32:e70026.
- Kui Du and Jia-Jun Fan
  TriCG with deflated restarting for symmetric quasi-definite linear systems.
  In preparation, 2025.

Thanks!