Deflation techniques for two classes of structured linear systems

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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

  FOR-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 $r = \mathrm{rank}(\mathbf{H}^{-1}\mathbf{S})$ 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

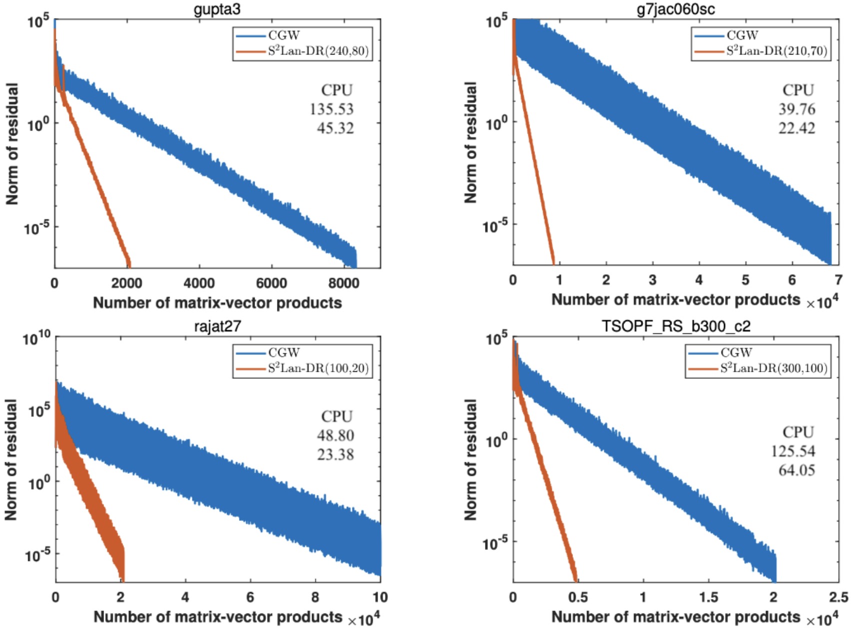
- S^{2}Lan-DR$(m, 2k)$

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

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. $\mathbf{S^2}$Lan-DR$(m, 2k)$



Rapoport with deflated restarting

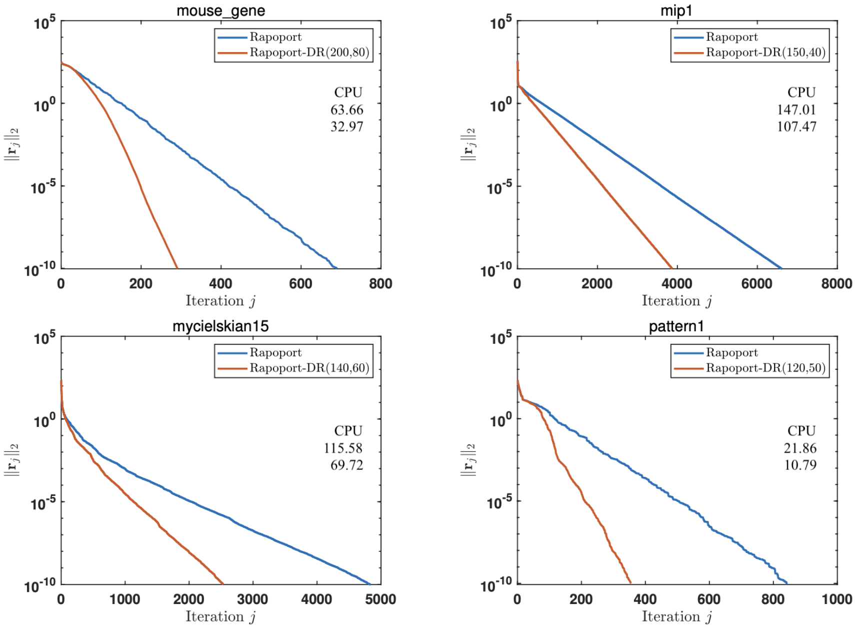
- Rapoport-DR$(m, 2k)$

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

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 $\mathbf{\Sigma} = \mathrm{diag}(\sigma_1, \ldots, \sigma_p)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, $p = \min(m, n)$, 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 $r = \mathrm{rank}(\mathbf{A})$):

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

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

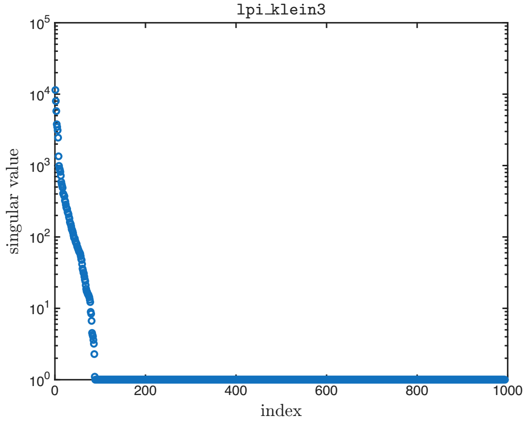
$$\begin{bmatrix} \mathbf{x}_j^{(i)} \\ \mathbf{y}_j^{(i)} \end{bmatrix} = \begin{bmatrix} \mathbf{U}_j^{(i)} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_j^{(i)} \end{bmatrix} \begin{bmatrix} \mathbf{I}_j & \mathbf{T}_j^{(i)} \\ (\mathbf{T}_j^{(i)})^\top & -\mathbf{I}_j \end{bmatrix}^{-1} \begin{bmatrix}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

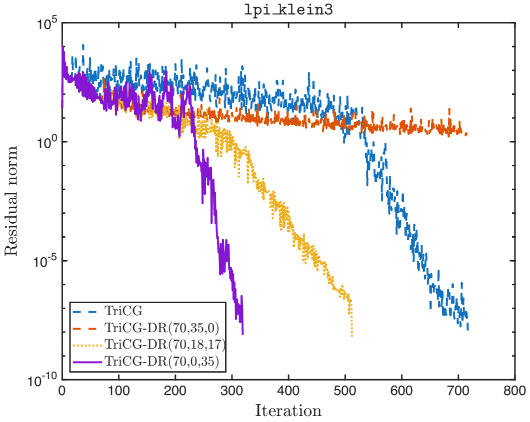
  which satisfies the Galerkin condition

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

- Using an $\text{LDL}^\top$ 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!