TriCG with deflated restarting for symmetric quasi-definite linear systems

Kui Du

kuidu@xmu.edu.cn

School of Mathematical Sciences, Xiamen University

https://kuidu.github.io

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Outline

1. Symmetric quasi-definite (SQD) linear systems
2. TriCG for SQD linear systems
3. TriCG with deflated restarting
4. Summary

Symmetric quasi-definite (SQD) 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 $\mathbf{c} \in \mathbb{R}^{n}$:

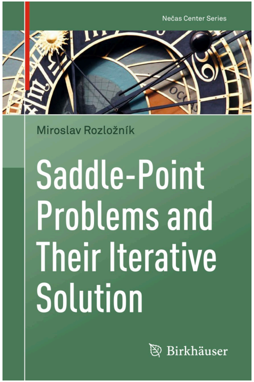
$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}, \quad \mathbf{H} = \begin{bmatrix} \mathbf{M} & \\ & \mathbf{N} \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix}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

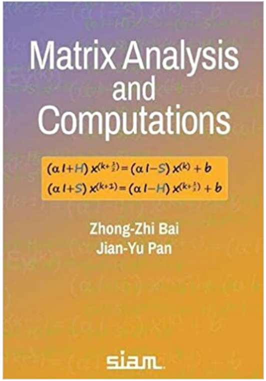
- Numerical optimization and numerical PDE, etc.
- Symmetric, indefinite, nonsingular
- Monolithic solvers: solving the system as a whole, for example, SYMMLQ, MINRES.

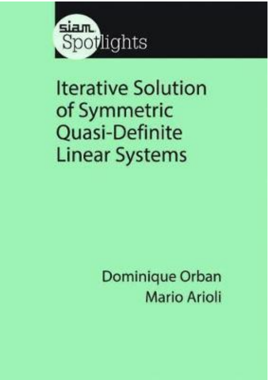
  Segregated solvers: exploiting the block structure, for example, TriCG, TriMR

Review paper and books

- Michele Benzi, Gene H. Golub, and Jörg Liesen
  Numerical solution of saddle point problems. Acta Numerica (2005).
- Books







The generalized Saunders–Simon–Yip tridiagonalization

- The generalized Saunders–Simon–Yip tridiagonalization:

$$\begin{aligned}
\mathbf{A}\mathbf{V}_k &= \mathbf{M}\mathbf{U}_{k+1}\mathbf{T}_{k+1,k} = \mathbf{M}\mathbf{U}_k\mathbf{T}_k + \beta_{k+1}\mathbf{M}\mathbf{u}_{k+1}\mathbf{e}_k^\top, \\
\mathbf{A}^\top\mathbf{U}_k &= \mathbf{N}\mathbf{V}_{k+1}\mathbf{T}_{k,k+1}^\top = \mathbf{N}\mathbf{V}_k\mathbf{T}_k^\top + \gamma_{k+1}\mathbf{N}\mathbf{v}_{k+1}\mathbf{e}_k^\top, \\
\mathbf{U}_{k+1}^\top\mathbf{M}\mathbf{U}_{k+1} &= \mathbf{V}_{k+1}^\top\mathbf{N}\mathbf{V}_{k+1} = \mathbf{I}_{k+1},
\end{aligned}$$

where

$$\mathbf{U}_k = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_k \end{bmatrix}, \quad \mathbf{V}_k = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_k \end{bmatrix},$$

and

$$\mathbf{T}_k = \mathrm{tridiag}(\beta_i, \alpha_i, \gamma_{i+1}), \quad \mathbf{T}_{k+1,k} = \begin{bmatrix} \mathbf{T}_k \\ \beta_{k+1}\mathbf{e}_k^\top \end{bmatrix}, \quad \mathbf{T}_{k,k+1} = \begin{bmatrix} \mathbf{T}_k & \gamma_{k+1}\mathbf{e}_k \end{bmatrix}.$$

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 $\mathbf{U}_k$, $\mathbf{V}_k$, and $\mathbf{T}_k$ are well defined. The kth TriCG iterate is

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

which satisfies the Galerkin condition

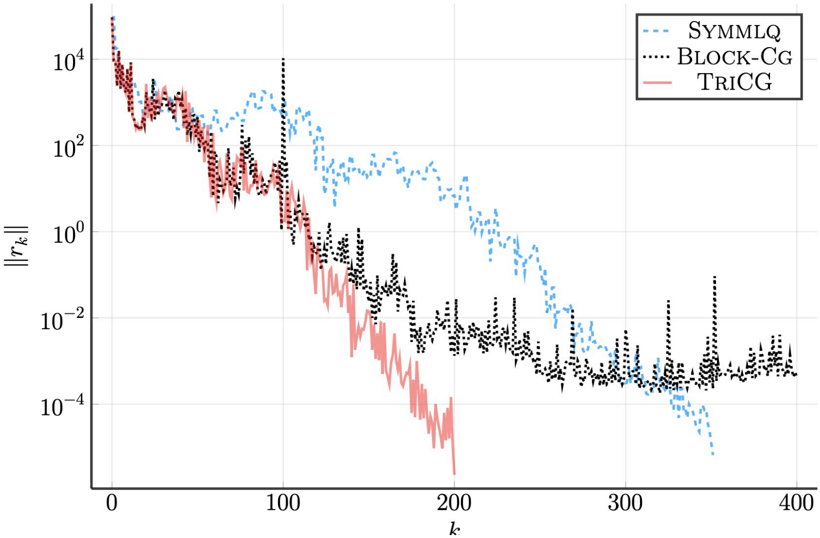
$$\begin{bmatrix} \mathbf{U}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_k \end{bmatrix}^\top \left(\begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix} - \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^\top & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x}_k \\ \mathbf{y}_k \end{bmatrix}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

- TriCG is faster than SYMMLQ and is 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)

Example: $\mathrm{M} = \mathrm{I}$, $\mathrm{N} = \mathrm{I}$, $\mathbf{A} =$ `lp_osa_07`



Elliptic singular value decomposition (ESVD)

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

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

  where $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1, \ldots, \sigma_p)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, $p = \min(m, n)$, 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)

Linear systems, Krylov subspace methods, and deflation

- Linear systems of equations

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

- Acceleration techniques for Krylov subspace methods

  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)

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

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

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

- Least squares or SP problems: Golub–Kahan + augmentation + restart
  Augmented LSQR (Baglama, Reichel, and Richmond, NA, 2013)
  Augmented CRAIG (Dumitrasc, Kruse, and Rüde, SIMAX, 2024)

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

A gSSY process with deflated restarting

- gSSY-DR(p,k):
$$\mathbf{A}\mathbf{V}_p^{(i)} = \mathbf{M}\mathbf{U}_p^{(i)}\mathbf{T}_p^{(i)} + \beta_{p+1}^{(i)}\mathbf{M}\mathbf{u}_{p+1}^{(i)}\mathbf{e}_p^\top,$$
$$\mathbf{A}^\top\mathbf{U}_p^{(i)} = \mathbf{N}\mathbf{V}_p^{(i)}(\mathbf{T}_p^{(i)})^\top + \gamma_{p+1}^{(i)}\mathbf{N}\mathbf{v}_{p+1}^{(i)}\mathbf{e}_p^\top.$$
For $i = 2, 3, \ldots,$
$$\mathbf{T}_p^{(i)} = \begin{bmatrix} \alpha_1^{(i)} & & & \gamma_2^{(i)} & & & \\ & \ddots & & \vdots & & & \\ & & \ddots & \gamma_{k+1}^{(i)} & & & \\ \beta_2^{(i)} & \cdots & \beta_{k+1}^{(i)} & \alpha_{k+1}^{(i)} & \gamma_{k+2}^{(i)} & & \\ & & & \beta_{k+2}^{(i)} & \alpha_{k+2}^{(i)} & \ddots & \\ & & & & \ddots & \ddots & \gamma_p^{(i)} \\ & & & & & \beta_p^{(i)} & \alpha_p^{(i)} \end{bmatrix}.$$

TriCG with deflated restarting

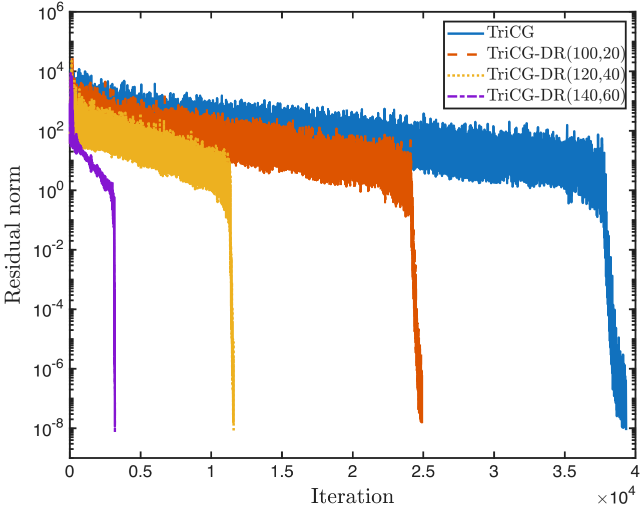
- The recurrences in the first cycle are the same as that of TriCG. Now consider cycle $i \geq 2$. The jth ($k+1 \leq j \leq p$) TriCG-DR(p,k) iterate is

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

  which satisfies the Galerkin condition.
- 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 $k+1 \leq j \leq p$.
- If the target k approximate elliptic singular triplets are sufficiently accurate, we stop restarting. In other words, the last cycle is implemented completely until a sufficiently accurate approximate solution is found or the maximum number of iterations is reached. Partial reorthogonalization is required.

Numerical experiment I

$$\mathbf{M} = \mathbf{I},\ \mathbf{N} = \mathbf{I},\ \mathbf{A} = \mathrm{diag}([\mathtt{linspace}(0, 800, 2000), \mathtt{linspace}(1e3, 1e5, 60)]);$$



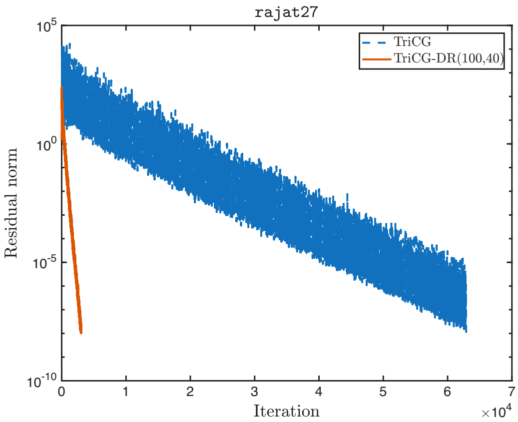
Numerical experiment II

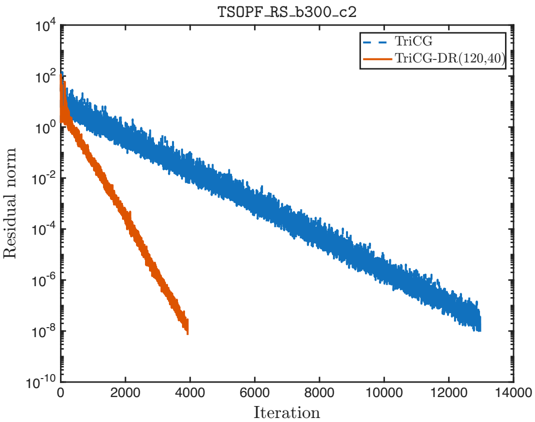
$\mathbf{M} = \mathbf{I}$, $\mathbf{N} = \mathbf{I}$, $\mathbf{A}$ is from the SuiteSparse Matrix Collection.

Table: The information of square matrices from the SuiteSparse Matrix Collection, runtime of TriCG and TriCG-DR, and values of parameters p and k of TriCG-DR.

Matrix	Size	Nnz	TriCG	TriCG-DR		
			Time(s)	Time(s)	p	k
gupta3	16783	9323427	17.55	7.61	240	120
g7jac060sc	17730	183325	16.82	10.10	60	20
rajat27	20640	97353	24.70	6.42	100	40
TSOPF_RS_b300_c2	28338	2943887	30.48	17.64	120	40

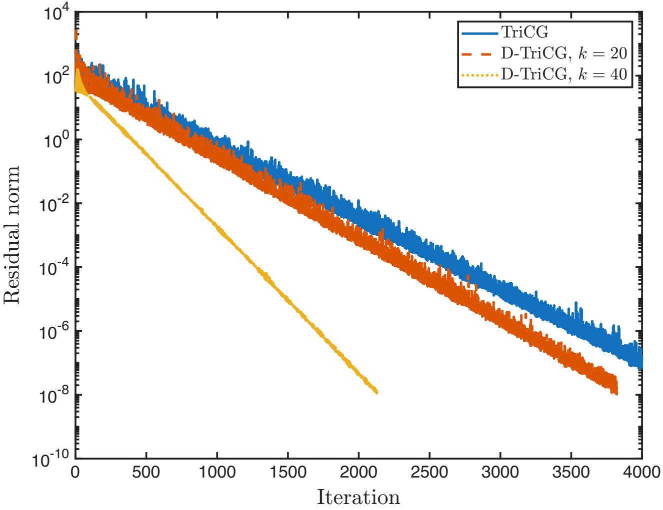
Numerical experiment II





Numerical experiment III

$$\mathbf{M} = \mathbf{I},\ \mathbf{N} = \mathbf{I},\ \mathbf{A} = \mathrm{diag}([\texttt{linspace}(0, 100, 1960), \texttt{linspace}(1000, 1020, 40)]);$$



Numerical experiment IV

- The matrices are obtained via IFISS on the test problem `channel_domain` for the unsteady incompressible Stokes equation.

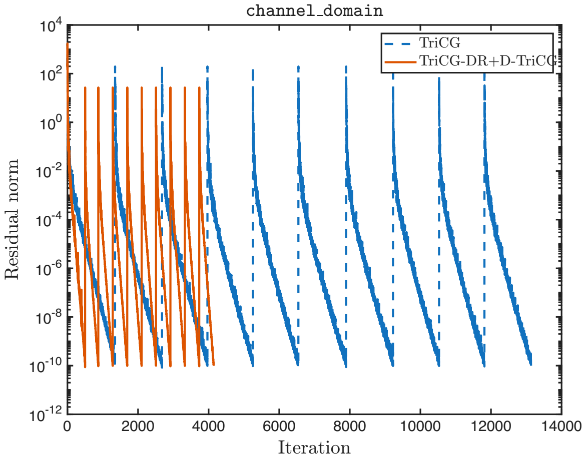
CPU time

TriCG

163.42

TriCG-DR+D-TriCG

108.85



Summary

- We have proposed gSSY-DR for computing partial spectral information.
- Based on gSSY-DR, we have proposed TriCG-DR for solving SQD linear systems. The new method has faster convergence and demonstrates a significant advantage in computational time.
- We have designed TriCG-DR+D-TRiCG for solving SQD linear systems with sequential multiple right-hand sides. Significant convergence acceleration is observed.

Thanks!