On Krylov subspace methods for skew-symmetric and shifted skew-symmetric linear systems

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joint work with J.-J. Fan, X.-H. Sun, F. Wang, Y.-L. Zhang

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Main references

- C. Greif, C.C. Paige, D. Titley-Peloquin and J. M. Varah
  Numerical equivalences among Krylov subspace algorithms for skew-symmetric matrices
  SIMAX 2016, 37(3), pp. 1071–1087
- C. Greif and J. M. Varah
  Iterative solution of skew-symmetric linear systems
  SIMAX 2009, 31(2), pp. 584–601
- E. Jiang
  Algorithm for solving shifted skew-symmetric linear system
  Frontiers of Mathematics in China 2007, 2(2), pp. 227–242

Outline

1. Preliminaries
2. Krylov subspace methods for skew-symmetric linear systems
3. Krylov subspace methods for shifted skew-symmetric linear systems
4. Summary and future work

Krylov subspaces and Arnoldi process

- Krylov subspaces for $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{b} \in \mathbb{R}^n$:

$$\mathcal{K}_k(\mathbf{A}, \mathbf{b}) := \mathrm{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \cdots, \mathbf{A}^{k-1}\mathbf{b}\}.$$

- The grade of $\mathbf{b}$ with respect to $\mathbf{A}$ is ℓ that satisfies

$$\dim \mathcal{K}_k(\mathbf{A}, \mathbf{b}) = \begin{cases} k, & \text{if } 1 \leq k \leq \ell, \\ \ell, & \text{if } k \geq \ell + 1. \end{cases}$$

- Arnoldi relation:

$$\mathbf{A}\mathbf{W}_k = \mathbf{W}_{k+1}\mathbf{H}_{k+1,k}, \quad \mathbf{H}_k = \mathbf{W}_k^\top \mathbf{A}\mathbf{W}_k, \quad 1 \leq k \leq \ell - 1,$$

$$\mathbf{A}\mathbf{W}_\ell = \mathbf{W}_\ell \mathbf{H}_\ell, \quad \mathbf{W}_\ell^\top \mathbf{W}_\ell = \mathbf{I}_\ell.$$

Krylov subspace methods for $\mathrm{Ax} = \mathrm{b}$ with $\mathrm{x}_0 = 0$

- GMRES and MINRES:

$$\mathbf{r}_k \perp \mathbf{A}\mathcal{K}_k(\mathbf{A}, \mathbf{b}) \quad \Leftrightarrow \quad \mathbf{x}_k = \underset{\mathbf{x} \in \mathcal{K}_k(\mathbf{A}, \mathbf{b})}{\operatorname{argmin}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2.$$

- FOM and CG:

$$\mathbf{r}_k \perp \mathcal{K}_k(\mathbf{A}, \mathbf{b}) \quad \Leftrightarrow \quad \mathbf{x}_k = \|\mathbf{b}\|_2 \mathbf{W}_k \mathbf{H}_k^{-1} \mathbf{e}_1.$$

- SYMMLQ:

$$\mathbf{x}_k = \underset{\mathbf{x} \in \mathcal{K}_k(\mathbf{A}, \mathbf{b})}{\operatorname{argmin}} \|\mathbf{x}\|_2 \quad \text{subject to} \quad \mathbf{b} - \mathbf{A}\mathbf{x} \perp \mathcal{K}_{k-1}(\mathbf{A}, \mathbf{b}).$$

- QR, LU, and LQ factorizations

Yousef Saad. *Iterative Methods for Sparse Linear Systems*, 2nd edition, SIAM, 2003.

Golub–Kahan bidiagonalization

Algorithm: GKB for $\mathbf{A} \in \mathbb{R}^{n\times m}$, $\mathbf{b} \in \mathbb{R}^n$

Compute $\beta_1 \mathbf{u}_1 := \mathbf{b}$ and $\alpha_1 \mathbf{v}_1 := \mathbf{A}^\top \mathbf{u}_1$.

for $j = 1, 2, \cdots$ **do**

$\beta_{j+1}\mathbf{u}_{j+1} := \mathbf{A}\mathbf{v}_j - \alpha_j \mathbf{u}_j$;

$\alpha_{j+1}\mathbf{v}_{j+1} := \mathbf{A}^\top \mathbf{u}_{j+1} - \beta_{j+1}\mathbf{v}_j$;

end

$$\mathbf{A}\mathbf{V}_j = \mathbf{U}_{j+1}\mathbf{B}_{j+1,j} = \mathbf{U}_j\mathbf{B}_j + \beta_{j+1}\mathbf{u}_{j+1}\mathbf{e}_j^\top,$$
$$\mathbf{A}^\top\mathbf{U}_{j+1} = \mathbf{V}_{j+1}\mathbf{B}_{j+1}^\top = \mathbf{V}_j\mathbf{B}_{j+1,j}^\top + \alpha_{j+1}\mathbf{v}_{j+1}\mathbf{e}_{j+1}^\top,$$
$$\mathbf{U}_j^\top\mathbf{U}_j = \mathbf{V}_j^\top\mathbf{V}_j = \mathbf{I}_j,$$
$$\mathrm{range}(\mathbf{U}_j) = \mathcal{K}_j(\mathbf{A}\mathbf{A}^\top, \mathbf{b}), \quad \mathrm{range}(\mathbf{V}_j) = \mathcal{K}_j(\mathbf{A}^\top\mathbf{A}, \mathbf{A}^\top\mathbf{b}).$$

CRAIG, LSQR, LSMR, LSLQ, LNLQ

- The normal equations (NE)

$$\mathbf{A}^\top \mathbf{A}\mathbf{x} = \mathbf{A}^\top \mathbf{b}$$

- The normal equations of the second kind (NE2)

$$\mathbf{A}\mathbf{A}^\top \mathbf{y} = \mathbf{b}, \quad \mathbf{x} = \mathbf{A}^\top \mathbf{y}$$

- CRAIG (1955, also called CGNE) "=" CG for NE2
- LSQR (1982) "=" CG for NE or MINRES for NE2
- LSMR (2011) "=" MINRES for NE
- LSLQ (2019) "=" SYMMLQ for NE
- LNLQ (2019) "=" SYMMLQ for NE2

Saunders–Simon–Yip tridiagonalization

Algorithm: SSY for $\mathbf{A} \in \mathbb{R}^{n\times m}$, $\mathbf{b} \in \mathbb{R}^n$, and $\mathbf{c} \in \mathbb{R}^m$

Set $\mathbf{u}_0 = \mathbf{0}$, $\mathbf{v}_0 = \mathbf{0}$. Compute $\beta_1 \mathbf{u}_1 := \mathbf{b}$ and $\alpha_1 \mathbf{v}_1 := \mathbf{c}$.

for $k = 1, 2, \cdots$ **do**

$\quad \mathbf{q} := \mathbf{A}\mathbf{v}_k - \alpha_k \mathbf{u}_{k-1}$; $\theta_k := \mathbf{u}_k^\top \mathbf{q}$;

$\quad \beta_{k+1}\mathbf{u}_{k+1} := \mathbf{q} - \theta_k \mathbf{u}_k$;

$\quad \alpha_{k+1}\mathbf{v}_{k+1} := \mathbf{A}^\top \mathbf{u}_k - \beta_k \mathbf{v}_{k-1} - \theta_k \mathbf{v}_k$;

end

$$\mathbf{A}\mathbf{V}_k = \mathbf{U}_{k+1}\mathbf{T}_{k+1,k} = \mathbf{U}_k\mathbf{T}_k + \beta_{k+1}\mathbf{u}_{k+1}\mathbf{e}_k^\top,$$

$$\mathbf{A}^\top\mathbf{U}_k = \mathbf{V}_{k+1}\mathbf{T}_{k,k+1}^\top = \mathbf{V}_k\mathbf{T}_k^\top + \alpha_{k+1}\mathbf{v}_{k+1}\mathbf{e}_k^\top,$$

$$\mathbf{U}_k^\top\mathbf{U}_k = \mathbf{V}_k^\top\mathbf{V}_k = \mathbf{I}_k, \quad \mathbf{T}_k = \mathbf{U}_k^\top\mathbf{A}\mathbf{V}_k.$$

USYMLQ, USYMQR

- C. C. Paige and M. A. Saunders

  Solution of Sparse Indefinite Systems of Linear Equations

  SINUM 1975, 12(4), pp. 617–629

- M. A. Saunders, H. D. Simon and E. L. Yip

  Two conjugate-gradient-type methods for unsymmetric linear equations

  SINUM 1988, 25(4), pp. 927–940

- USYMLQ and USYMQR are in the same fashion as SYMMLQ and MINRES.

- If $\mathbf{A}^\top = -\mathbf{A}$ and $\mathbf{c} = \mathbf{b}$, then SSY = Arnoldi = skew-Lanczos.

skew-Lanczos

- $\mathbf{A}^\top = -\mathbf{A}$ (skew-symmetric), skew-Lanczos, $\mathbf{H}_k^\top = -\mathbf{H}_k$

$$\mathbf{H}_{k+1,k} = \begin{bmatrix} 0 & -\gamma_2 & & \\ \gamma_2 & 0 & \ddots & \\ & \ddots & \ddots & -\gamma_k \\ & & \gamma_k & 0 \\ & & & \gamma_{k+1} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_k \\ \gamma_{k+1}\mathbf{e}_k^\top \end{bmatrix}.$$

Theorem

Assume that $\mathbf{A}^\top = -\mathbf{A}$. For each j with $1 \leq j \leq \ell/2$, $\mathbf{H}_{2j}$ is nonsingular. If $\mathbf{b} \in \mathrm{range}(\mathbf{A})$, then ℓ is even and $\mathbf{H}_\ell$ is nonsingular. Otherwise, ℓ is odd and $\mathbf{H}_\ell$ is singular.

- one step of Golub–Kahan = two steps of skew-Lanczos

S^2CG and CRAIG for skew-symmetric systems

- CG-type solution (if any):

$$\mathbf{x}_k = \|\mathbf{b}\|_2 \mathbf{W}_k \mathbf{H}_k^{-1} \mathbf{e}_1.$$

- For nonsingular skew-symmetric systems, S^2CG of Greif and Varah computes the even iterates $\mathbf{x}_{2j}^{\mathrm{G}}$ and returns $\mathbf{A}^{-1}\mathbf{b}$ in exact arithmetic.

Proposition

Assume that $\mathbf{A}$ is a singular skew-symmetric matrix, and that $\mathbf{b} \in \mathrm{range}(\mathbf{A})$. Let $\mathbf{x}_j^{\mathrm{G}}$ and $\mathbf{x}_j^{\mathrm{CRAIG}}$ be the jth iterates of S^2CG and CRAIG for $\mathbf{A}\mathbf{x} = \mathbf{b}$, respectively. For each $1 \le j \le \ell/2$, we have $\mathbf{x}_{2j}^{\mathrm{G}} = \mathbf{x}_j^{\mathrm{CRAIG}}$. Moreover, S^2CG returns $\mathbf{A}^{\dagger}\mathbf{b}$.

S^2MR and LSQR for skew-symmetric systems

- Greif and Varah (2009) proposed S^2MR for a nonsingular skew-symmetric system. Greif et al. (2016) showed that

$$\mathbf{x}_{2j}^{\mathrm{M}} = \mathbf{x}_{2j+1}^{\mathrm{M}} = \mathbf{x}_j^{\mathrm{LSQR}}.$$

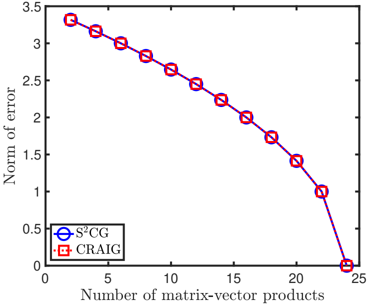
Proposition

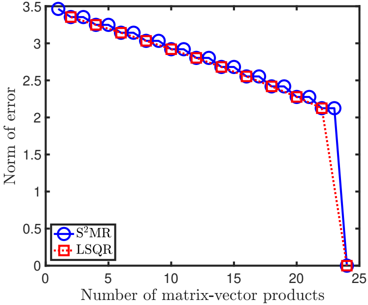
Assume that $\mathbf{A}$ is a singular skew-symmetric matrix. Let $\mathbf{x}_j^{\mathrm{M}}$ and $\mathbf{x}_j^{\mathrm{LSQR}}$ be the jth iterates of S^2MR and LSQR for $\mathbf{A}\mathbf{x} = \mathbf{b}$, respectively. For each j with $\mathbf{x}_j^{\mathrm{LSQR}} \neq \mathbf{A}^\dagger \mathbf{b}$, i.e., LSQR does not converge at the jth iteration, we have $\mathbf{x}_{2j}^{\mathrm{M}} = \mathbf{x}_{2j+1}^{\mathrm{M}} = \mathbf{x}_j^{\mathrm{LSQR}}$. Whether $\mathbf{A}\mathbf{x} = \mathbf{b}$ is consistent or not, S^2MR always returns the pseudoinverse solution $\mathbf{A}^\dagger \mathbf{b}$.

Numerical experiments

- A singular consistent skew-symmetric system $\mathbf{Sx} = \mathbf{b}$ with

$$\mathbf{S} = \begin{bmatrix} 0 & 1 & & \\ -1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & -1 & 0 \end{bmatrix} \in \mathbb{R}^{n\times n}, \quad \mathbf{b} = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ \vdots \\ 0 \\ -1/\sqrt{2} \end{bmatrix} \in \mathbb{R}^{n}.$$

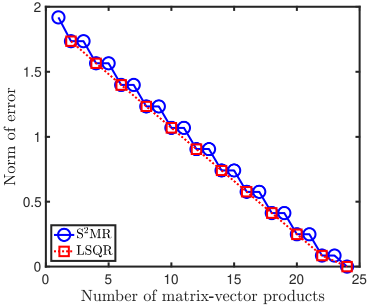




Numerical experiments

- A singular inconsistent skew-symmetric system $\mathbf{Sx} = \mathbf{b}$ with

$$\mathbf{S} = \begin{bmatrix} 0 & 1 & & \\ -1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & -1 & 0 \end{bmatrix} \in \mathbb{R}^{n\times n}, \quad \mathbf{b} = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ \vdots \\ 0 \\ 1/\sqrt{2} \end{bmatrix} \in \mathbb{R}^{n}.$$



The convergence for $\mathbf{A}^{\dagger}\mathbf{b}$ when $\mathbf{A}^{\top} = -\mathbf{A}$

Summary of the convergence of different methods for $\mathbf{A}^{\dagger}\mathbf{b}$ of all types of skew-symmetric linear systems. Y means the algorithm is convergent and N means not.

Method	singular consistent	singular inconsistent	nonsingular
S^{2}CG	Y	N	Y
S^{2}MR	Y	Y	Y
CRAIG	Y	N	Y
LSQR	Y	Y	Y
LSMR	Y	Y	Y
LSLQ	Y	Y	Y
LNLQ	Y	N	Y

Shifted skew-symmetric systems

- Assume that $\mathbf{A} = \alpha\mathbf{I} + \mathbf{S}$ with $\alpha \neq 0$ and $\mathbf{S}^\top = -\mathbf{S}$.
- Arnoldi relation:

$$\mathbf{W}_\ell^\top \mathbf{W}_\ell = \mathbf{I}_\ell, \quad \mathbf{S}\mathbf{W}_\ell = \mathbf{W}_\ell \mathbf{H}_\ell, \quad \mathbf{H}_\ell = \mathbf{W}_\ell^\top \mathbf{S}\mathbf{W}_\ell.$$

$$\mathbf{A}\mathbf{W}_\ell = \alpha\mathbf{W}_\ell + \mathbf{W}_\ell\mathbf{H}_\ell = \mathbf{W}_\ell\mathbf{T}_\ell, \quad \mathbf{T}_\ell := \alpha\mathbf{I}_\ell + \mathbf{H}_\ell.$$

Proposition

GKB applied to $\mathbf{A} = \alpha\mathbf{I} + \mathbf{S}$ and $\mathbf{b}$ must stop in $\ell_0 = \lceil \ell/2 \rceil$ steps with $\alpha_{\ell_0} > 0$ and $\beta_{\ell_0+1} = 0$. For each j with $1 \leq j \leq \ell_0 - 1$, we have $\alpha_j > \gamma_{2j}$ and $\beta_{j+1} = \gamma_{2j+1}\gamma_{2j}/\alpha_j < \gamma_{2j+1}$.

- S^{3}LQ, S^{3}CG, S^{3}MR via LQ, LU, and QR factorizations.

$\mathrm{S^3CG}$ (a special case of CGW)

Algorithm: $\mathrm{S^3CG}$ for shifted skew-symmetric systems

Set $\mathbf{x}_0^{\mathrm{G}} = \mathbf{0}$, $\mathbf{r}_0^{\mathrm{G}} = \mathbf{b}$ and $\mathbf{p}_0^{\mathrm{G}} = \mathbf{r}_0^{\mathrm{G}}$;

for $k = 1, 2, \ldots,$ **do** until convergence:

$$\alpha_k^{\mathrm{G}} = \frac{(\mathbf{r}_{k-1}^{\mathrm{G}})^\top \mathbf{r}_{k-1}^{\mathrm{G}}}{(\mathbf{p}_{k-1}^{\mathrm{G}})^\top \mathbf{A}\mathbf{p}_{k-1}^{\mathrm{G}}};$$

$$\mathbf{x}_k^{\mathrm{G}} = \mathbf{x}_{k-1}^{\mathrm{G}} + \alpha_k^{\mathrm{G}} \mathbf{p}_{k-1}^{\mathrm{G}};$$

$$\mathbf{r}_k^{\mathrm{G}} = \mathbf{r}_{k-1}^{\mathrm{G}} - \alpha_k^{\mathrm{G}} \mathbf{A}\mathbf{p}_{k-1}^{\mathrm{G}};$$

$$\beta_k^{\mathrm{G}} = -\frac{(\mathbf{r}_k^{\mathrm{G}})^\top \mathbf{r}_k^{\mathrm{G}}}{(\mathbf{r}_{k-1}^{\mathrm{G}})^\top \mathbf{r}_{k-1}^{\mathrm{G}}};$$

$$\mathbf{p}_k^{\mathrm{G}} = \mathbf{r}_k^{\mathrm{G}} + \beta_k^{\mathrm{G}} \mathbf{p}_{k-1}^{\mathrm{G}};$$

end

S^{3}CG: properties

Proposition

Let S^{3}CG be applied to a shifted skew-symmetric matrix problem $\mathbf{A}\mathbf{x} = \mathbf{b}$. In exact arithmetic, as long as the algorithm has not yet converged $($i.e., $\mathbf{r}^{\mathrm{G}}_{k-1} \neq \mathbf{0})$, it proceeds without breaking down, and we have the following identities of subspaces:

$$\begin{aligned}\mathcal{K}_k(\mathbf{A}, \mathbf{b}) &= \mathrm{span}\{\mathbf{x}^{\mathrm{G}}_1, \mathbf{x}^{\mathrm{G}}_2, \cdots, \mathbf{x}^{\mathrm{G}}_k\} \\ &= \mathrm{span}\{\mathbf{p}^{\mathrm{G}}_0, \mathbf{p}^{\mathrm{G}}_1, \cdots, \mathbf{p}^{\mathrm{G}}_{k-1}\} \\ &= \mathrm{span}\{\mathbf{r}^{\mathrm{G}}_0, \mathbf{r}^{\mathrm{G}}_1, \cdots, \mathbf{r}^{\mathrm{G}}_{k-1}\}.\end{aligned}$$

The residuals are mutually orthogonal, $(\mathbf{r}^{\mathrm{G}}_i)^\top \mathbf{r}^{\mathrm{G}}_k = 0$ for $i \neq k$, and the search directions are "semiconjugate", $(\mathbf{p}^{\mathrm{G}}_i)^\top \mathbf{A}\mathbf{p}^{\mathrm{G}}_k = 0$ for $i < k$.

S^3CG: optimality and convergence

- S^3CG has the optimality properties

$$\|\mathbf{x}_{2k}^{\mathrm{G}} - \mathbf{A}^{-1}\mathbf{b}\|_2 = \min_{\mathbf{x}\in\mathbf{A}^\top\mathcal{K}_{2k}(\mathbf{A},\mathbf{b})} \|\mathbf{x} - \mathbf{A}^{-1}\mathbf{b}\|_2,$$

  and

$$\|\mathbf{x}_{2k+1}^{\mathrm{G}} - \mathbf{A}^{-1}\mathbf{b}\|_2 = \min_{\mathbf{x}\in\mathbf{b}/\alpha+\mathbf{A}^\top\mathcal{K}_{2k+1}(\mathbf{A},\mathbf{b})} \|\mathbf{x} - \mathbf{A}^{-1}\mathbf{b}\|_2.$$

- Let $\beta = \|\mathbf{S}\|_2$. Then

$$\frac{\|\mathbf{x}_{2k}^{\mathrm{G}} - \mathbf{A}^{-1}\mathbf{b}\|_2}{\|\mathbf{A}^{-1}\mathbf{b}\|_2} \leq 2\left(\frac{\sqrt{1+|\beta/\alpha|^2}-1}{\sqrt{1+|\beta/\alpha|^2}+1}\right)^k.$$

  The same bound holds for $\|\mathbf{x}_{2k+1}^{\mathrm{G}} - \mathbf{A}^{-1}\mathbf{b}\|_2/\|\mathbf{x}_1^{\mathrm{G}} - \mathbf{A}^{-1}\mathbf{b}\|_2$. The bound indicates that a "fast" convergence of S^3CG can be expected when $|\beta/\alpha| > 0$ is "small".

S^{3}CG: relation to CRAIG

Lemma

Let $\mathbf{A} = \alpha\mathbf{I} + \mathbf{S}$ *be a shifted skew-symmetric matrix. The subspaces* $\mathbf{A}^\top\mathcal{K}_k(\mathbf{S}^2, \mathbf{b})$ *and* $\mathbf{A}^\top\mathcal{K}_k(\mathbf{S}^2, \mathbf{S}\mathbf{b})$ *are orthogonal, and the solution* $\mathbf{A}^{-1}\mathbf{b}$ *is orthogonal to* $\mathbf{A}^\top\mathcal{K}_k(\mathbf{S}^2, \mathbf{S}\mathbf{b})$*.*

Theorem

Let $\mathbf{A} = \alpha\mathbf{I} + \mathbf{S}$ *be a shifted skew-symmetric matrix. Let* $\mathbf{x}_k^{\mathrm{G}}$ *and* $\mathbf{x}_k^{\mathrm{CRAIG}}$ *be the* k*th iterates of S*^{3}*CG and CRAIG for* $\mathbf{A}\mathbf{x} = \mathbf{b}$*, respectively. Then we have*

$$\mathbf{x}_{2k}^{\mathrm{G}} = \mathbf{x}_k^{\mathrm{CRAIG}}.$$

$\mathrm{S^3MR}$ (see Jiang 2007)

- The kth iterate: $\mathbf{x}_k^{\mathrm{M}} = \underset{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})}{\operatorname{argmin}} \|\mathbf{b}-\mathbf{A}\mathbf{x}\|_2$.
- $\mathrm{S^3MR}$ does not stagnate, i.e., $\|\mathbf{r}_k^{\mathrm{M}}\|_2$ is strictly decreasing.

$$\frac{\|\mathbf{r}_k^{\mathrm{M}}\|_2}{\|\mathbf{b}\|_2} \leq 2\left(\frac{|\beta/\alpha|}{\sqrt{1+|\beta/\alpha|^2}+1}\right)^k.$$

Proposition

Let $\mathbf{A}=\alpha\mathbf{I}+\mathbf{S}$ and $\alpha\neq 0$. For each k with $1\leq k\leq \ell_0-1$, it holds that

$$\|\mathbf{b}-\mathbf{A}\mathbf{x}_{2k}^{\mathrm{M}}\|_2 \leq \|\mathbf{b}-\mathbf{A}\mathbf{x}_k^{\mathrm{LSQR}}\|_2.$$

Moreover, we have $\mathbf{x}_\ell^{\mathrm{M}}=\mathbf{x}_{\ell_0}^{\mathrm{LSQR}}=\mathbf{A}^{-1}\mathbf{b}$.

- Numerical experiments: $\|\mathbf{b}-\mathbf{A}\mathbf{x}_{2k}^{\mathrm{M}}\|_2 < \|\mathbf{b}-\mathbf{A}\mathbf{x}_k^{\mathrm{LSQR}}\|_2$.

S^{3}MR

Algorithm: S^{3}MR for shifted skew-symmetric systems

Set $\mathbf{x}_0^{\mathrm{M}} = \mathbf{0}$, $\widetilde{\delta}_1 = \alpha$, $c_0 = 1$, $\mathbf{w}_0 = \mathbf{0}$, $\gamma_1 \mathbf{w}_1 = \mathbf{b}$, and $\widetilde{\psi}_1 = \gamma_1$;

for $k = 1, 2, \ldots,$ **do** until convergence:

$\gamma_{k+1}\mathbf{w}_{k+1} := \mathbf{S}\mathbf{w}_k + \gamma_k \mathbf{w}_{k-1}$;

$\delta_k = \sqrt{\widetilde{\delta}_k^2 + \gamma_{k+1}^2}$, $c_k = \widetilde{\delta}_k/\delta_k$, $s_k = \gamma_{k+1}/\delta_k$;

$\widetilde{\delta}_{k+1} = \alpha c_k + \gamma_{k+1} c_{k-1} s_k$, $\psi_k = c_k \widetilde{\psi}_k$, $\widetilde{\psi}_{k+1} = -s_k \widetilde{\psi}_k$;

if $k \leq 2$ **then**

$\mathbf{p}_k = \mathbf{w}_k/\delta_k$;

else

$\mathbf{p}_k = (\mathbf{w}_k + \gamma_k s_{k-2} \mathbf{p}_{k-2})/\delta_k$;

end

$\mathbf{x}_k^{\mathrm{M}} = \mathbf{x}_{k-1}^{\mathrm{M}} + \psi_k \mathbf{p}_k$;

end

S^3LQ

- The kth iterate:

$$\mathbf{x}_k^{\mathrm{L}} := \underset{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})}{\operatorname{argmin}} \|\mathbf{x}\|_2 \quad \text{subject to} \quad \mathbf{b}-\mathbf{A}\mathbf{x} \perp \mathcal{K}_{k-1}(\mathbf{A},\mathbf{b}).$$

Theorem

For $k > 1$, we have $\mathbf{x}_k^{\mathrm{L}} = \underset{\mathbf{x}\in\mathbf{A}^\top\mathcal{K}_{k-1}(\mathbf{A},\mathbf{b})}{\operatorname{argmin}} \|\mathbf{x}-\mathbf{A}^{-1}\mathbf{b}\|_2$.

Theorem

Let $\mathbf{x}_k^{\mathrm{L}}$ and $\mathbf{x}_k^{\mathrm{G}}$ be the iterates generated at iteration k of S^3LQ and S^3CG, respectively. As long as the algorithms have not yet converged, we have $\mathbf{x}_{2j}^{\mathrm{L}} = \mathbf{x}_{2j+1}^{\mathrm{L}} = \mathbf{x}_{2j}^{\mathrm{G}}$ for $j \geq 1$.

$\mathbf{S^3LQ}$

Algorithm: $\mathrm{S^3LQ}$ for shifted skew-symmetric systems

Set $\mathbf{x}_1^{\mathrm{L}} = \mathbf{0}$, $\widetilde{\delta}_1 = \alpha$, $s_{-1} = 1$, $\xi_{-1} = -1$, $s_0 = 0$,

$\xi_0 = 0$, $c_0 = 1$, $\gamma_1 = \|\mathbf{b}\|_2$;

Set $\mathbf{w}_0 = \mathbf{0}$, $\mathbf{w}_1 = \mathbf{b}/\gamma_1$, and $\widetilde{\mathbf{p}}_1 = \mathbf{w}_1$;

for $k = 1, 2, \ldots,$ **do** until convergence:

$\gamma_{k+1}\mathbf{w}_{k+1} := \mathbf{S}\mathbf{w}_k + \gamma_k \mathbf{w}_{k-1}$;

$\delta_k = \sqrt{\widetilde{\delta}_k^2 + \gamma_{k+1}^2}$, $c_k = \widetilde{\delta}_k/\delta_k$, $s_k = -\gamma_{k+1}/\delta_k$;

$\widetilde{\delta}_{k+1} = \alpha c_k - \gamma_{k+1} c_{k-1} s_k$; $\xi_k = -\gamma_k s_{k-2}\xi_{k-2}/\delta_k$;

$\mathbf{p}_k = c_k \widetilde{\mathbf{p}}_k + s_k \mathbf{w}_{k+1}$;

$\mathbf{x}_{k+1}^{\mathrm{L}} = \mathbf{x}_k^{\mathrm{L}} + \xi_k \mathbf{p}_k$; $\quad \widetilde{\mathbf{p}}_{k+1} = c_k \mathbf{w}_{k+1} - s_k \widetilde{\mathbf{p}}_k$

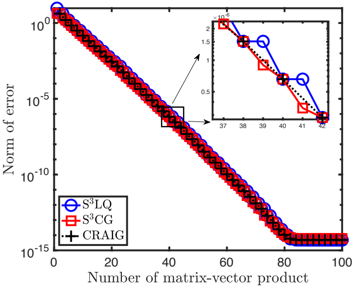
end

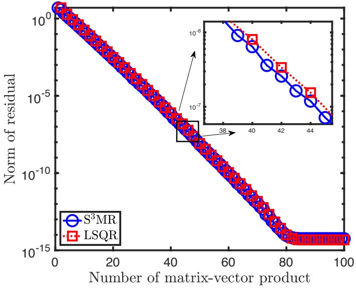
Numerical experiments

- Consider $\mathbf{S} = \mathbf{I}_m \otimes \mathbf{S}_m(\sigma_1) + \mathbf{S}_m(\sigma_2) \otimes \mathbf{I}_m$,

$$\mathbf{S}_m(\sigma) = \begin{bmatrix} 0 & \sigma & & \\ -\sigma & 0 & \ddots & \\ & \ddots & \ddots & \sigma \\ & & -\sigma & 0 \end{bmatrix} \in \mathbb{R}^{m\times m}.$$

Set $m = 15$, $\alpha = 0.8$, $\sigma_1 = 0.4$, and $\sigma_2 = 0.6$.

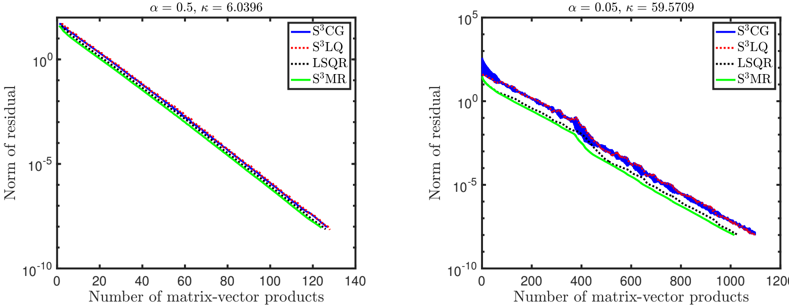




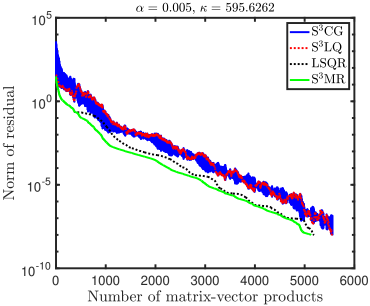
Numerical experiments

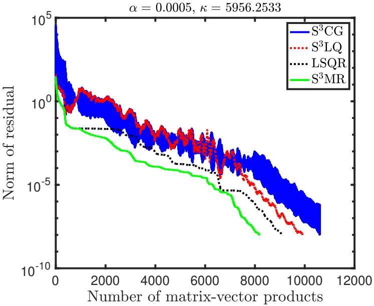
- $m = 25$, $\sigma_1 = 0.4$, $\sigma_2 = 0.5$, $\sigma_3 = 0.6$

$$\mathbf{S} = \mathbf{I}_m \otimes \mathbf{I}_m \otimes \mathbf{S}_m(\sigma_1) + \mathbf{I}_m \otimes \mathbf{S}_m(\sigma_2) \otimes \mathbf{I}_m + \mathbf{S}_m(\sigma_3) \otimes \mathbf{I}_m \otimes \mathbf{I}_m$$



Numerical experiments





Summary and future work

- We extend the results of Greif et al. (SIMAX 2016) to singular skew-symmetric linear systems.
- We systematically study three Krylov subspace methods (called S^{3}CG, S^{3}MR, and S^{3}LQ) for solving shifted skew-symmetric linear systems. We provide relations among the three methods and those based on GKB and SSY.

- Effects of finite precision
- Preconditioning techniques
- More general cases: $\mathbf{I}$ replaced by an SPD matrix
- $\ldots$

Our paper and slides

- K. Du, J.-J. Fan, X.-H. Sun, F. Wang, and Y.-L. Zhang.
  On Krylov subspace methods for skew-symmetric and shifted skew-symmetric linear systems.
  Advances in Computational Mathematics (2024) 50:78

- The slides are available at
  https://kuidu.github.io/talk.html

Thanks!