RSMAR: An iterative method for range-symmetric 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

Numerical Algebra @ BNU Zhuhai on 03/30/2024

Two main references

- A. Montoison, D. Orban, and M. A. Saunders.
  MINARES: An iterative solver for symmetric linear systems.
  arXiv:2310.01757, 2023.

- Y. Liu, A. Milzarek, and F. Roosta.
  Obtaining pseudo-inverse solutions with MINRES.
  arXiv:2309.17096, 2023.

Outline

1. The pseudoinverse solution of range-symmetric systems
2. GMRES-type methods for singular range-symmetric systems
3. RSMAR for range-symmetric systems
4. Numerical experiments
5. Summary

The pseudoinverse solution

- $\mathbf{Ax} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{m \times n}, \quad \mathbf{b} \in \mathbb{R}^m.$
  Consistent if $\mathbf{b} \in \mathrm{range}(\mathbf{A})$, otherwise, inconsistent.
- $\mathbf{A}^\dagger$: the Moore–Penrose inverse of $\mathbf{A}$
- $\mathbf{A}^\dagger\mathbf{b}$: the pseudoinverse solution

$\mathbf{Ax} = \mathbf{b}$	$\mathrm{rank}(\mathbf{A})$	$\mathbf{A}^\dagger\mathbf{b}$
consistent	$= n$	unique solution
consistent	$< n$	unique minimum 2-norm solution
inconsistent	$= n$	unique least-squares (LS) solution
inconsistent	$< n$	unique minimum 2-norm LS solution

Krylov subspaces and (least squares) solutions

- $\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{n \times n}, \quad \mathbf{b},\ \mathbf{x}_0 \in \mathbb{R}^n, \quad \mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0,$

$$\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) := \mathrm{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0\}.$$

- ℓ: the grade of $\mathbf{r}_0$ with respect to $\mathbf{A}$, i.e., ℓ satisfies

$$\dim \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) = \begin{cases} k, & \text{if } k \le \ell, \\ \ell, & \text{if } k \ge \ell + 1. \end{cases}$$

- For any $\mathbf{A} \in \mathbb{R}^{n \times n}$,
  (i) $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$: $\#$ LS solution in $\mathbf{x}_0 + \mathcal{K}_{\ell-1}(\mathbf{A}, \mathbf{r}_0) \le 1$;
  (ii) $\mathbf{b} \in \mathrm{range}(\mathbf{A})$: $\#$ solution in $\mathbf{x}_0 + \mathcal{K}_{\ell}(\mathbf{A}, \mathbf{r}_0) \le 1$.

Range-symmetric systems

- range-symmetric $\mathbf{A}$: $\quad \mathrm{range}(\mathbf{A}) = \mathrm{range}(\mathbf{A}^\top).$

Fact I:

$$\mathbf{A} = \mathbf{U}\begin{bmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\mathbf{U}^\top.$$

($\mathbf{C}$ is invertible and $\mathbf{U}$ is orthogonal.)

Fact II:

$$\mathbf{A}^\dagger = \mathbf{A}^{\mathrm{D}} = \mathbf{U}\begin{bmatrix} \mathbf{C}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\mathbf{U}^\top. \quad \text{(Drazin inverse)}$$

Fact III:

$$\begin{aligned} \mathbf{A}^\dagger\mathbf{b} + \mathrm{null}(\mathbf{A}) &= \{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}^\top\mathbf{A}\mathbf{x} = \mathbf{A}^\top\mathbf{b}\} \\ &= \{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}^2\mathbf{x} = \mathbf{A}\mathbf{b}\}. \end{aligned}$$

GMRES for singular range-symmetric systems

- GMRES: $\mathbf{x}_k := \underset{\mathbf{x}\in\mathbf{x}_0+\mathcal{K}_k(\mathbf{A},\mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{b}-\mathbf{A}\mathbf{x}\|.$
- For singular range-symmetric $\mathbf{A}$ [BW97]:

  (i) $\mathbf{b} \in \operatorname{range}(\mathbf{A})$: $\mathbf{x}_\ell =$ solution. More precisely,

  $$\mathbf{x}_\ell = \mathbf{A}^\dagger\mathbf{b} + (\mathbf{I}-\mathbf{A}^\dagger\mathbf{A})\mathbf{x}_0,$$

  the orthogonal projection of $\mathbf{x}_0$ onto the solution set

  $$\{\mathbf{x}\in\mathbb{R}^n : \mathbf{A}\mathbf{x}=\mathbf{b}\} = \mathbf{A}^\dagger\mathbf{b} + \operatorname{null}(\mathbf{A}).$$

  (ii) $\mathbf{b} \notin \operatorname{range}(\mathbf{A})$: $\mathbf{x}_{\ell-1} =$ LS solution. Which one?

[BW97] P. N. Brown and H. F. Walker. *GMRES on (nearly) singular systems*. SIMAX, 1997.

GMRES for singular (skew-)symmetric systems

- "(skew-)symmetric" $\in$ "range-symmetric"
- For symmetric $\mathbf{A}$, if $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, then $\mathbf{x}_{\ell-1}$ = LS solution, but not necessarily $\mathbf{A}^\dagger\mathbf{b}$ [CPS11].
  MINRES-QLP or MINRES with a lifting strategy.
- For skew-symmetric $\mathbf{A}$, i.e., $\mathbf{A}^\top = -\mathbf{A}$, if $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, then

$$\mathbf{r}_{\ell-1}^\top(\mathbf{x}_{\ell-1} - \mathbf{x}_0) = 0,$$

  which implies

$$\mathbf{x}_{\ell-1} = \mathbf{A}^\dagger\mathbf{b} + (\mathbf{I} - \mathbf{A}^\dagger\mathbf{A})\mathbf{x}_0.$$

[CPS11] S.-C. T. Choi, C. C. Paige, and M. A. Saunders. *MINRES-QLP: A Krylov subspace method for indefinite or singular symmetric systems*. SISC, 2011.

A lifting strategy [LMR23]

- If $\operatorname{range}(\mathbf{A}) = \operatorname{range}(\mathbf{A}^\top)$ and $\mathbf{b} \notin \operatorname{range}(\mathbf{A})$, then the lifted vector,

$$\widetilde{\mathbf{x}}_{\ell-1} := \mathbf{x}_{\ell-1} - \frac{\mathbf{r}_{\ell-1}^\top(\mathbf{x}_{\ell-1} - \mathbf{x}_0)}{\mathbf{r}_{\ell-1}^\top \mathbf{r}_{\ell-1}} \mathbf{r}_{\ell-1},$$

  is the orthogonal projection of $\mathbf{x}_0$ onto the least squares solution set $\{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}^\top \mathbf{A}\mathbf{x} = \mathbf{A}^\top \mathbf{b}\}$, i.e.,

$$\widetilde{\mathbf{x}}_{\ell-1} = \mathbf{A}^\dagger \mathbf{b} + (\mathbf{I} - \mathbf{A}^\dagger \mathbf{A})\mathbf{x}_0.$$

- $\mathbf{x}_0 = \mathbf{0} \;\Rightarrow\; \widetilde{\mathbf{x}}_{\ell-1} = \mathbf{A}^\dagger \mathbf{b}$.

[LMR23] Y. Liu, A. Milzarek, and F. Roosta. *Obtaining pseudo-inverse solutions with MINRES*. arXiv:2309.17096, 2023.

Summary of GMRES-type methods

- Let $\mathbf{A}$ be range-symmetric. For simplicity, we set $\mathbf{x}_0 = \mathbf{0}$.

Method	Minimization property at step k
GMRES	$\mathbf{x}_k := \operatorname{argmin}_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})} \\|\mathbf{b}-\mathbf{A}\mathbf{x}\\|$
RRGMRES	$\mathbf{x}_k^{\mathrm{R}} := \operatorname{argmin}_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{A}\mathbf{b})} \\|\mathbf{b}-\mathbf{A}\mathbf{x}\\|$
DGMRES	$\mathbf{x}_k^{\mathrm{D}} := \operatorname{argmin}_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{A}\mathbf{b})} \\|\mathbf{A}(\mathbf{b}-\mathbf{A}\mathbf{x})\\|$
RSMAR	$\mathbf{x}_k^{\mathrm{A}} := \operatorname{argmin}_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})} \\|\mathbf{A}(\mathbf{b}-\mathbf{A}\mathbf{x})\\|$

Consistent: $\mathbf{x}_\ell = \mathbf{x}_\ell^{\mathrm{R}} = \mathbf{x}_\ell^{\mathrm{D}} = \mathbf{A}^\dagger\mathbf{b}$, $\quad \mathbf{x}_\ell^{\mathrm{A}} = ???$

Inconsistent: $\widetilde{\mathbf{x}}_{\ell-1} = \mathbf{x}_{\ell-1}^{\mathrm{R}} = \mathbf{x}_{\ell-1}^{\mathrm{D}} = \mathbf{A}^\dagger\mathbf{b}$, $\quad \mathbf{x}_{\ell-1}^{\mathrm{A}} = ???$

[MOS23] A. Montoison, D. Orban, and M. A. Saunders. *MINARES: An iterative solver for symmetric linear systems.* arXiv:2310.01757, 2023.

RSMAR for range-symmetric systems

- RSMAR: $\mathbf{x}_k^{\mathrm{A}} := \underset{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})}{\operatorname{argmin}} \|\mathbf{A}(\mathbf{b}-\mathbf{A}\mathbf{x})\|$, (well-defined?)

- For range-symmetric $\mathbf{A}$, if $\mathbf{b} \in \mathrm{range}(\mathbf{A})$, then $\mathbf{x}_\ell^{\mathrm{A}} = \mathbf{x}_\ell$, and if $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, then $\mathbf{x}_{\ell-1}^{\mathrm{A}} = \mathbf{x}_{\ell-1}$. In other words, the final iterates of GMRES and RSMAR are the same.

- For inconsistent systems, $\|\mathbf{r}_{\ell-1}\| \neq 0$, but $\|\mathbf{A}\mathbf{r}_{\ell-1}\| = 0$.

- RSMAR for $\mathbf{A}\mathbf{x} = \mathbf{b}$ "$=$" GMRES for $\mathbf{A}\mathbf{y} = \mathbf{A}\mathbf{b}$, $\mathbf{y} = \mathbf{A}\mathbf{x}$:

$$\min_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})} \|\mathbf{A}(\mathbf{b}-\mathbf{A}\mathbf{x})\| = \min_{\mathbf{y}\in\mathcal{K}_k(\mathbf{A},\mathbf{A}\mathbf{b})} \|\mathbf{A}\mathbf{b}-\mathbf{A}\mathbf{y}\|,$$

$$\mathbf{y}_k = \mathbf{A}\mathbf{x}_k^{\mathrm{A}} = \underset{\mathbf{y}\in\mathcal{K}_k(\mathbf{A},\mathbf{A}\mathbf{b})}{\operatorname{argmin}} \|\mathbf{A}\mathbf{b}-\mathbf{A}\mathbf{y}\|.$$

Implementation I (inspired by simpler GMRES)

- Arnoldi process yields $\mathrm{span}\{\widehat{\mathbf{v}}_1, \widehat{\mathbf{v}}_2, \ldots, \widehat{\mathbf{v}}_k\} = \mathcal{K}_k(\mathbf{A}, \mathbf{Ab})$,

$$\widehat{\beta}_1 \widehat{\mathbf{v}}_1 = \mathbf{Ab}, \quad \mathbf{A}\widehat{\mathbf{V}}_k = \widehat{\mathbf{V}}_{k+1}\widehat{\mathbf{H}}_{k+1,k}, \quad \widehat{\mathbf{V}}_k^\top \widehat{\mathbf{V}}_k = \mathbf{I}_k.$$

- $\min\limits_{\mathbf{y}\in\mathcal{K}_k(\mathbf{A},\mathbf{Ab})} \|\mathbf{Ab} - \mathbf{Ay}\| = \min\limits_{\widehat{\mathbf{z}}\in\mathbb{R}^k} \|\widehat{\beta}_1 \mathbf{e}_1 - \widehat{\mathbf{H}}_{k+1,k}\widehat{\mathbf{z}}\| \;\Rightarrow$
  $\mathbf{y}_k = \widehat{\mathbf{V}}_k \widehat{\mathbf{z}}_k$ with $\widehat{\mathbf{z}}_k = \operatorname*{argmin}\limits_{\widehat{\mathbf{z}}\in\mathbb{R}^k} \|\widehat{\beta}_1 \mathbf{e}_1 - \widehat{\mathbf{H}}_{k+1,k}\widehat{\mathbf{z}}\|$.

- $\mathcal{K}_k(\mathbf{A}, \mathbf{b}) = \mathrm{span}\{\mathbf{b}, \widehat{\mathbf{v}}_1, \ldots, \widehat{\mathbf{v}}_{k-1}\}$ and $\mathbf{y}_k = \mathbf{A}\mathbf{x}_k^{\mathrm{A}} \;\Rightarrow$

$$\mathbf{x}_k^{\mathrm{A}} = \begin{bmatrix} \mathbf{b} & \widehat{\mathbf{V}}_{k-1} \end{bmatrix} \mathbf{z}_k,$$

  where $\mathbf{z}_k$ solves

$$\mathbf{A}\begin{bmatrix} \mathbf{b} & \widehat{\mathbf{V}}_{k-1} \end{bmatrix} \mathbf{z} = \widehat{\mathbf{V}}_k \begin{bmatrix} \widehat{\beta}_1 \mathbf{e}_1 & \widehat{\mathbf{H}}_{k,k-1} \end{bmatrix} \mathbf{z} = \widehat{\mathbf{V}}_k \widehat{\mathbf{z}}_k.$$

Implementation II (inspired by RRGMRES)

- Arnoldi process yields $\mathrm{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k\} = \mathcal{K}_k(\mathbf{A}, \mathbf{b})$,

$$\beta_1 \mathbf{v}_1 = \mathbf{b}, \quad \mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\mathbf{H}_{k+1,k}, \quad \mathbf{V}_k^\top \mathbf{V}_k = \mathbf{I}_k.$$

- The subproblem:

$$\begin{aligned} &\min_{\mathbf{x} \in \mathcal{K}_k(\mathbf{A},\mathbf{b})} \|\mathbf{A}(\mathbf{b} - \mathbf{A}\mathbf{x})\| \\ &\qquad = \min_{\mathbf{z} \in \mathbb{R}^k} \|\beta_1 \mathbf{H}_{k+2,k+1}\mathbf{e}_1 - \mathbf{H}_{k+2,k+1}\mathbf{H}_{k+1,k}\mathbf{z}\|. \end{aligned}$$

- Two QR factorizations are required:

$$\mathbf{H}_{k+1,k} = \mathbf{Q}_{k+1} \begin{bmatrix} \mathbf{R}_k \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{H}_{k+2,k+1}\mathbf{Q}_{k+1} \begin{bmatrix} \mathbf{I}_k \\ \mathbf{0} \end{bmatrix} = \widetilde{\mathbf{Q}}_{k+2} \begin{bmatrix} \widetilde{\mathbf{R}}_k \\ \mathbf{0} \end{bmatrix}.$$

- $\mathbf{x}_k^{\mathrm{A}} = \mathbf{V}_k \mathbf{R}_k^{-1} \widetilde{\mathbf{R}}_k^{-1} \begin{bmatrix} \mathbf{I}_k & \mathbf{0} \end{bmatrix} \widetilde{\mathbf{Q}}_{k+2}^\top \beta_1 (h_{11}\mathbf{e}_1 + h_{21}\mathbf{e}_2)$.

MINARES for symmetric systems [MOS23]

- GMRES for symmetric systems "$\Leftrightarrow$" MINRES
- RSMAR for symmetric systems "$\Leftrightarrow$" MINARES
- The MINARES implementation in [MOS23] is based on the Arnoldi relation $\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\mathbf{H}_{k+1,k}$, and thus can be viewed as a short recurrence variant of RSMAR-II.
- We derive a new implementation for MINARES, which is based on $\mathbf{A}\widehat{\mathbf{V}}_k = \widehat{\mathbf{V}}_{k+1}\widehat{\mathbf{H}}_{k+1,k}$ and can be viewed as a short recurrence variant of RSMAR-I.

[MOS23] A. Montoison, D. Orban, and M. A. Saunders. *MINARES: An iterative solver for symmetric linear systems.* arXiv:2310.01757, 2023.

Numerical experiments

- A boundary value problem

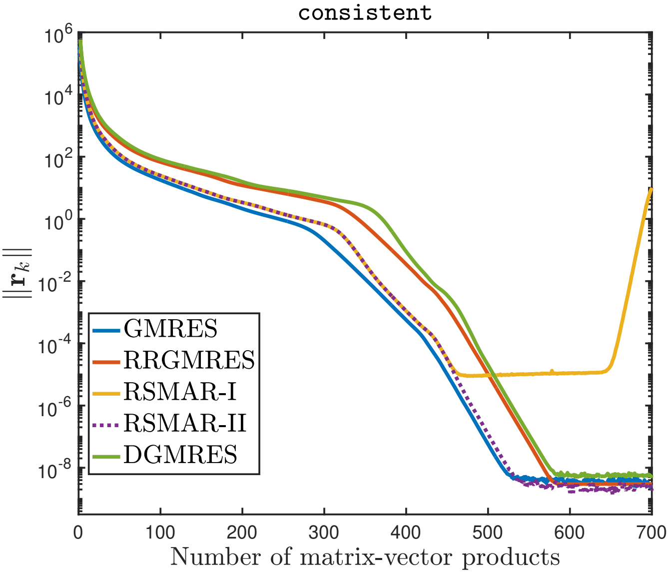
$$\begin{cases} \Delta u + d\dfrac{\partial u}{\partial x} = f, & \text{in} \quad \Omega := [0,1] \times [0,1], \\ u(x,0) = u(x,1), & \text{for} \quad 0 \le x \le 1, \\ u(0,y) = u(1,y), & \text{for} \quad 0 \le y \le 1, \end{cases}$$

  where d is a constant and f is a given function. [BW97]
- FD discretization yields a singular range-symmetric $\mathbf{A}$:

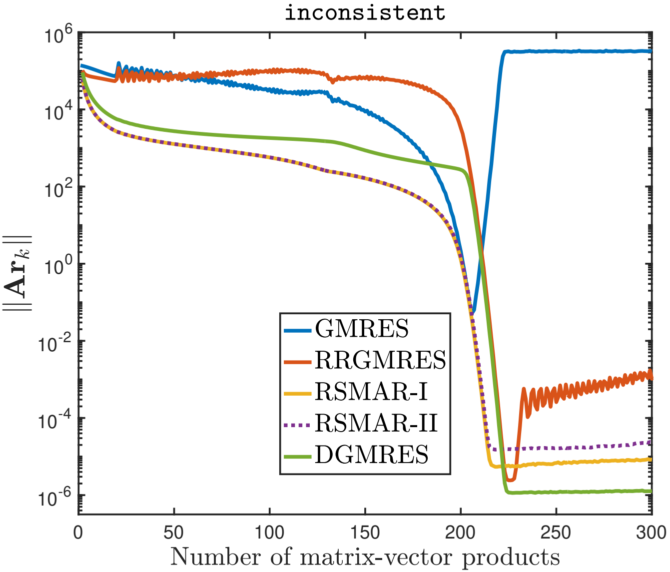
$$\mathbf{A} = \begin{bmatrix} \mathbf{T}_m & \mathbf{I}_m & & \mathbf{I}_m \\ \mathbf{I}_m & \ddots & \ddots & \\ & \ddots & \ddots & \mathbf{I}_m \\ \mathbf{I}_m & & \mathbf{I}_m & \mathbf{T}_m \end{bmatrix}, \quad \mathbf{T}_m = \begin{bmatrix} -4 & \alpha_+ & & \alpha_- \\ \alpha_- & \ddots & \ddots & \\ & \ddots & \ddots & \alpha_+ \\ \alpha_+ & & \alpha_- & -4 \end{bmatrix},$$

  where $m = 100$, $h = 1/m$, $\alpha_\pm = 1 \pm dh/2$, and $d = 10$.

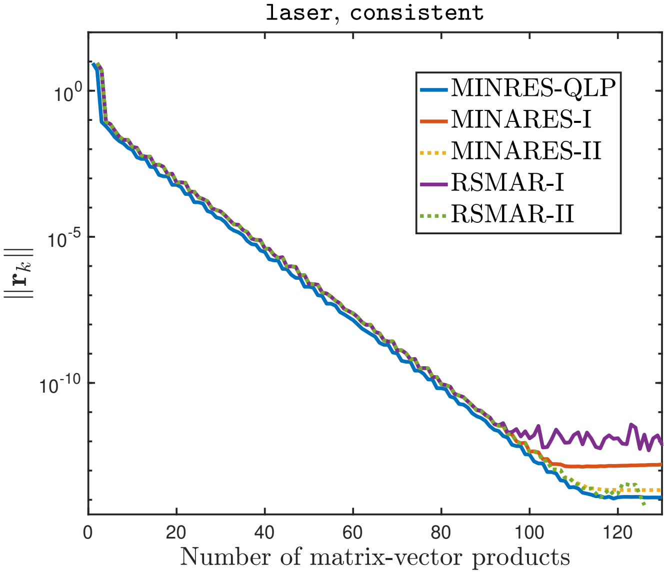
Example: a consistent range-symmetric system



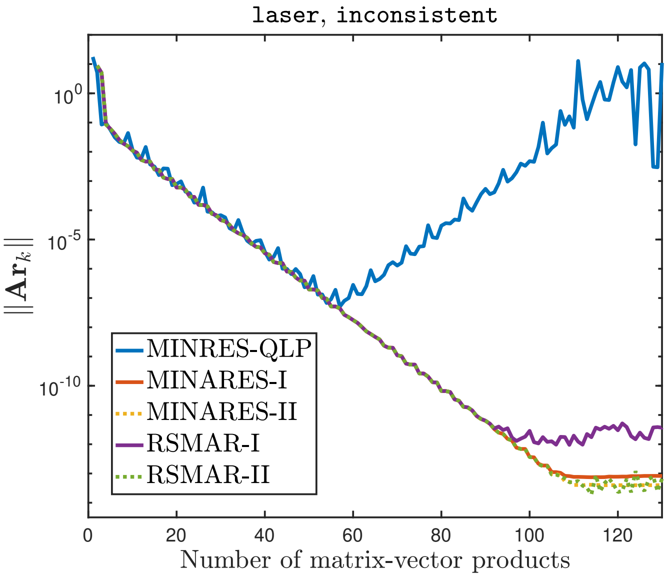
Example: an inconsistent range-symmetric system



Example: a consistent symmetric system



Example: an inconsistent symmetric system



Summary

- RSMAR enriches the family of Krylov subspace methods for range-symmetric systems.

- For range-symmetric systems, the final iterates of RSMAR and GMRES are the same.

- For range-symmetric $\mathbf{A}$, $\quad \mathbf{x}_0 = \mathbf{0}$,

  (i) $\mathbf{b} \in \mathrm{range}(\mathbf{A})$: the final iterate of RSMAR is $\mathbf{A}^\dagger \mathbf{b}$, and

  (ii) $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$: the final iterate of RSMAR is a least squares solution and a lifting strategy can be used to obtain $\mathbf{A}^\dagger \mathbf{b}$.

Summary

- On singular inconsistent range-symmetric systems, RSMAR outperforms GMRES, RRGMRES, and DGMRES, and thus should be the preferred method in finite precision arithmetic.

- RSMAR-II is better than RSMAR-I in finite precision arithmetic.

- Possible research directions:

  (1) preconditioning

  (2) stopping criteria

  (3) performance for linear discrete ill-posed problems

  ......

Our manuscript, slides, and MATLAB codes

- K. Du, J.-J. Fan, and F. Wang.
  Obtaining the pseudoinverse solution of singular range-symmetric linear systems with GMRES-type methods.
  arXiv:2401.11788, 2024.

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

- The MATLAB codes are available at
  `https://kuidu.github.io/code.html`