RSMAR: An iterative method for range-symmetric linear systems

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joint work with Jia-Jun Fan and Fang Wang

Beijing Normal University at 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. Preliminaries
2. GMRES-type methods for singular range-symmetric systems
3. Symmetric systems
4. Numerical experiments
5. Summary

The pseudoinverse solution

- $\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{m \times n}, \quad \mathbf{b} \in \mathbb{R}^m.$

  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

$\mathbf{A}\mathbf{x} = \mathbf{b}$	$\mathrm{rank}(\mathbf{A})$	$\mathbf{A}^\dagger\mathbf{b}$
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

Range-symmetric systems

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

Krylov subspaces

- $\mathbf{x}_0 \in \mathbb{R}^n$, $\quad \mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$,
- $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$: the kth Krylov subspace

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

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

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

- *If $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, there is at most one LS solution in $\mathbf{x}_0 + \mathcal{K}_{\ell-1}(\mathbf{A}, \mathbf{r}_0)$, and if $\mathbf{b} \in \mathrm{range}(\mathbf{A})$, at most one solution in $\mathbf{x}_0 + \mathcal{K}_\ell(\mathbf{A}, \mathbf{r}_0)$.*

GMRES for singular range-symmetric systems

- The kth approximate solution at step k of 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 $\mathbf{A}$ we have [BW97]:
(i) If $\mathbf{b} \in \operatorname{range}(\mathbf{A})$, then for all $0 \leq k \leq \ell - 1$, $\mathbf{x}_k$ is not a solution, and

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

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

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

(ii) If $\mathbf{b} \notin \operatorname{range}(\mathbf{A})$, then $\mathbf{x}_{\ell-1}$ is a least squares solution.

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

A lifting strategy [LMR23]

- $\mathbf{r}_{\ell-1} := \mathbf{b} - \mathbf{A}\mathbf{x}_{\ell-1}$.
- If $\mathrm{range}(\mathbf{A}) = \mathrm{range}(\mathbf{A}^\top)$ and $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, 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.,

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

- By using $\mathbf{x}_0 = \mathbf{0}$, we obtain the pseudoinverse solution $\mathbf{A}^\dagger\mathbf{b}$.

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

GMRES for (skew-)symmetric systems

- "(skew-)symmetric" $\in$ "range-symmetric"
- For symmetric $\mathbf{A}$, if $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, then $\mathbf{x}_{\ell-1}$ is a least squares solution, but not necessarily the pseudoinverse solution [CPS11].
- For skew-symmetric $\mathbf{A}$, i.e., $\mathbf{A}^\top = -\mathbf{A}$, if $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$, then

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

  This implies that if $\mathbf{x}_0 \in \mathrm{range}(\mathbf{A})$ then the $(\ell - 1)$th GMRES iterate

$$\mathbf{x}_{\ell-1} = \mathbf{A}^\dagger \mathbf{b}.$$

[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.

Summary of GMRES-type methods

- 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	$\mathbf{x}_k^{\mathrm{D}} := \operatorname{argmin}_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{A}\mathbf{b})} \|\mathbf{A}(\mathbf{b}-\mathbf{A}\mathbf{x})\|$

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

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

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

  MINARES [MOS23] for symmetric systems

RSMAR for range-symmetric systems

- RSMAR generates an approximation

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

  which is well defined for range-symmetric systems.
- For range-symmetric $\mathbf{A}$, if $\mathbf{b} \in \operatorname{range}(\mathbf{A})$, then $\mathbf{x}_\ell^{\mathrm{A}} = \mathbf{x}_\ell$, and if $\mathbf{b} \notin \operatorname{range}(\mathbf{A})$, then $\mathbf{x}_{\ell-1}^{\mathrm{A}} = \mathbf{x}_{\ell-1}$.

  In other words, for range-symmetric systems, GMRES and RSMAR terminate with the same (least squares) solution.
- RSMAR for $\mathbf{A}\mathbf{x} = \mathbf{b}$ "$=$" GMRES for $\mathbf{A}\mathbf{y} = \mathbf{A}\mathbf{b}, \mathbf{y} = \mathbf{A}\mathbf{x}$:

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

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

Implementation I (inspired by simpler GMRES)

- Arnoldi process for $\mathcal{K}_k(\mathbf{A}, \mathbf{Ab})$:

$$\widehat{\beta}_1 \widehat{\mathbf{v}}_1 = \mathbf{Ab}, \quad \mathbf{A}\widehat{\mathbf{V}}_k = \widehat{\mathbf{V}}_{k+1}\widehat{\mathbf{H}}_{k+1,k}, \quad \widehat{\mathbf{V}}_k^\top \widehat{\mathbf{V}}_k = \mathbf{I}_k,$$
$$\mathcal{K}_k(\mathbf{A}, \mathbf{Ab}) = \mathrm{span}\{\widehat{\mathbf{v}}_1, \widehat{\mathbf{v}}_2, \dots, \widehat{\mathbf{v}}_k\}.$$

- GMRES: $\min_{\mathbf{y} \in \mathcal{K}_k(\mathbf{A}, \mathbf{Ab})} \|\mathbf{Ab} - \mathbf{Ay}\| = \min_{\widehat{\mathbf{z}} \in \mathbb{R}^k} \|\widehat{\beta}_1 \mathbf{e}_1 - \widehat{\mathbf{H}}_{k+1,k}\widehat{\mathbf{z}}\|.$

  $\mathbf{y}_k = \mathbf{A}\mathbf{x}_k^{\mathrm{A}} = \widehat{\mathbf{V}}_k \widehat{\mathbf{z}}_k$ with $\widehat{\mathbf{z}}_k = \operatorname{argmin}_{\widehat{\mathbf{z}} \in \mathbb{R}^k} \|\widehat{\beta}_1 \mathbf{e}_1 - \widehat{\mathbf{H}}_{k+1,k}\widehat{\mathbf{z}}\|.$

- From $\mathcal{K}_k(\mathbf{A}, \mathbf{b}) = \mathrm{span}\{\mathbf{b}, \widehat{\mathbf{v}}_1, \dots, \widehat{\mathbf{v}}_{k-1}\}$, we have

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

  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 for $\mathcal{K}_k(\mathbf{A}, \mathbf{b})$:

$$\beta_1 \mathbf{v}_1 = \mathbf{b}, \quad \mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\mathbf{H}_{k+1,k}, \quad \mathbf{V}_k^\top \mathbf{V}_k = \mathbf{I}_k,$$
$$\mathcal{K}_k(\mathbf{A}, \mathbf{b}) = \operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k\}.$$

- The subproblem:

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

- Two QR factorizations are required:

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

Symmetric systems

- GMRES for symmetric systems "⇔" MINRES
- RSMAR for symmetric systems "⇔" MINARES [MOS23]
- The MINARES implementation in 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

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

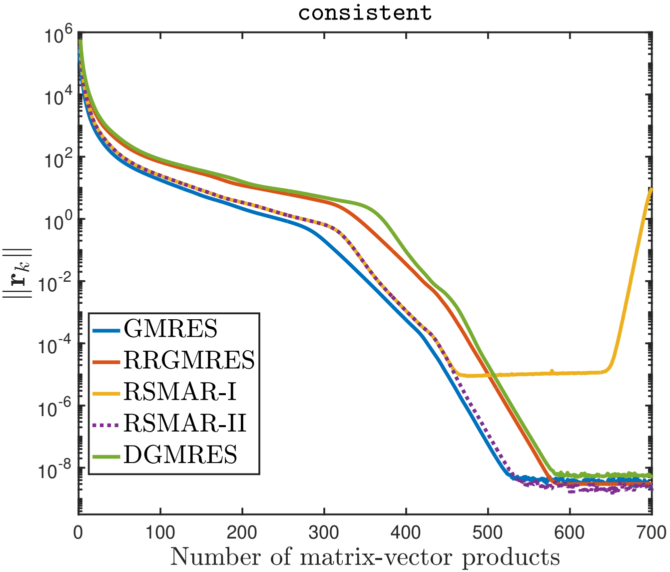
  where d is a constant and f is a given function.

- FD discretization yields a singular range-symmetric $\mathbf{A}$:

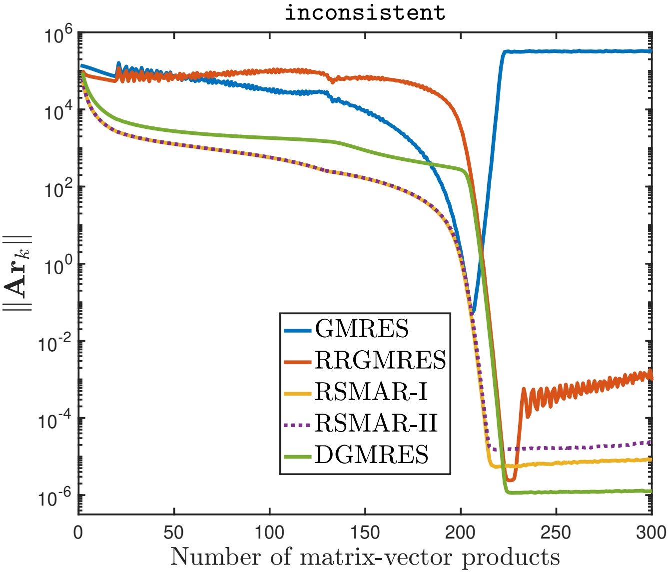
$$\mathbf{A} = \begin{bmatrix} \mathbf{T}_m & \mathbf{I}_m & & \mathbf{I}_m \\ \mathbf{I}_m & \ddots & \ddots & \\ & \ddots & \ddots & \mathbf{I}_m \\ \mathbf{I}_m & & \mathbf{I}_m & \mathbf{T}_m \end{bmatrix}, \quad \mathbf{T}_m = \begin{bmatrix} -4 & \alpha_+ & & \alpha_- \\ \alpha_- & \ddots & \ddots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

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

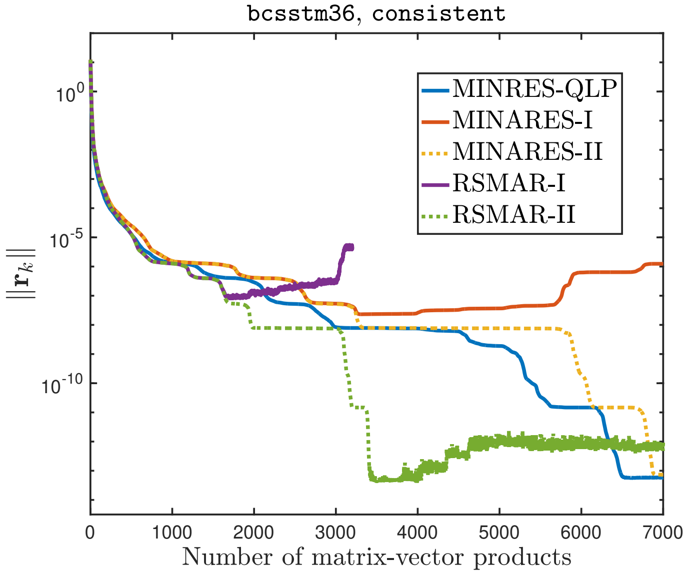
Convergence history for a consistent system



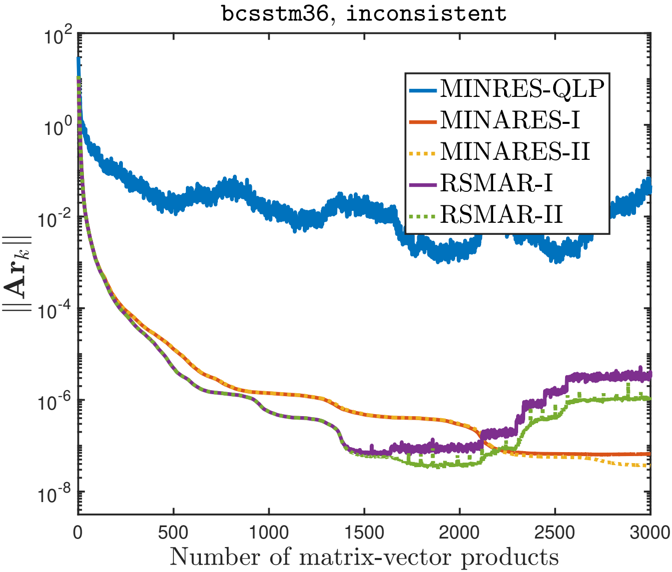
Convergence history for an inconsistent system



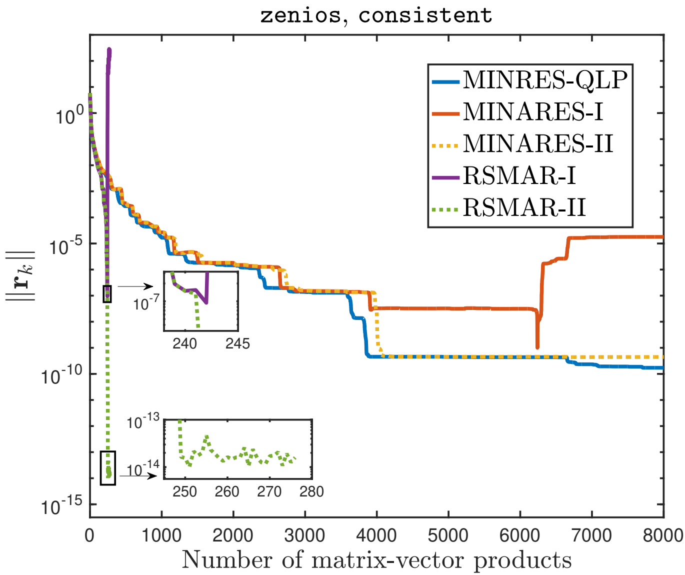
More numerical results



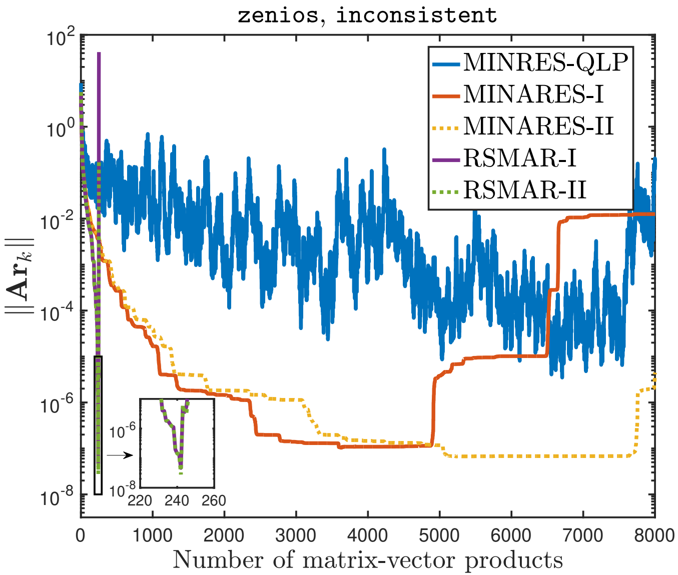
More numerical results



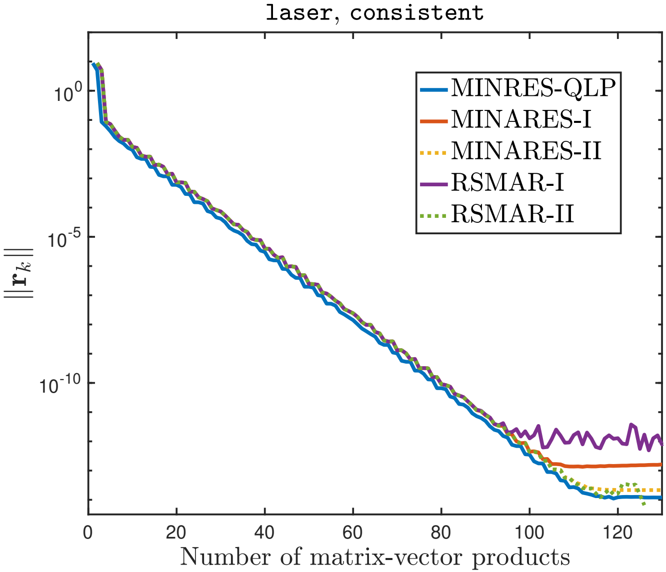
More numerical results



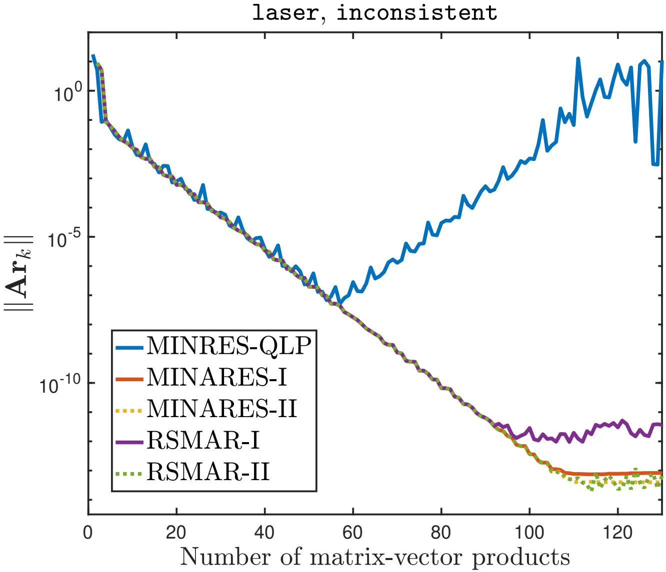
More numerical results



More numerical results



More numerical results



Summary

- RSMAR completes the family of Krylov subspace methods based on the Arnoldi process for range-symmetric linear systems.
- By minimizing the $\mathbf{A}$-residual norm $\|\mathbf{A}\mathbf{r}_k\|$ (which always converges to zero for range-symmetric $\mathbf{A}$), RSMAR can be applied to solve any range-symmetric systems.
- We have shown that in exact arithmetic, RSMAR and GMRES both determine the pseudoinverse solution if $\mathbf{b} \in \mathrm{range}(\mathbf{A})$, and terminate with the same least squares solution if $\mathbf{b} \notin \mathrm{range}(\mathbf{A})$.
- A lifting strategy can be used to obtain the pseudoinverse solution when the reached least squares solution is not.

Summary

- Our numerical experiments show that on singular inconsistent range-symmetric systems, RSMAR outperforms GMRES, RRGMRES, and DGMRES, and should be the preferred method in finite precision arithmetic.

- As for the implementation for RSMAR, RSMAR-II is better than RSMAR-I in finite precision arithmetic.

- Possible research directions:

  (1) preconditioning techniques

  (2) stopping criteria

  (3) performance for linear discrete ill-posed problems

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Manuscript and MATLAB codes

- Kui Du, Jia-Jun Fan, and Fang Wang.
  Obtaining the pseudoinverse solution of singular range-symmetric linear systems with GMRES-type methods.
  arXiv:2401.11788, 2024.

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

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