On some Krylov subspace methods tailored for large-scale block two-by-two linear systems

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joint work with Jia-Jun Fan and Fang Wang

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Outline

1. Block two-by-two linear systems
2. SPMR-SC, SPQMR-SC, nsLSQR
3. GPMR
4. Randomized Gram–Schmidt process, randomized GMRES
5. Sketched GMRES + k-truncated Arnoldi
6. Summary

Block two-by-two linear systems

- Nonsymmetric saddle-point linear systems of the form:

$$\begin{bmatrix} \mathbf{M} & \mathbf{A}^\top \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{b} \end{bmatrix},$$

  where $\mathbf{M} \in \mathbb{R}^{m \times m}$ is invertible, $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times m}$ are nonzero, and $\mathbf{b} \in \mathbb{R}^n$ is nonzero.

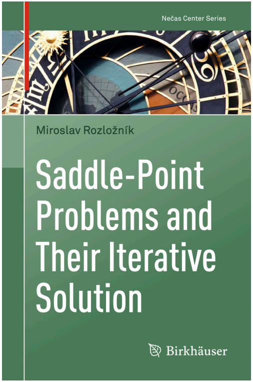
- Nonsymmetric partitioned linear systems of the form:

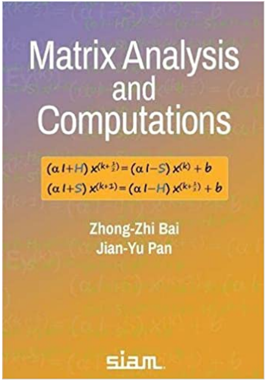
$$\begin{bmatrix} \lambda\mathbf{I} & \mathbf{A} \\ \mathbf{B} & \mu\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix},$$

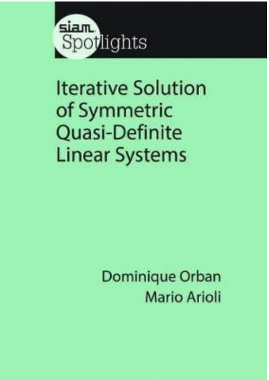
  where $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times m}$, and $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{c} \in \mathbb{R}^n$. Note that λ and/or μ may be zero.

Review papers and books

- Michele Benzi, Gene H. Golub, and Jörg Liesen
  Numerical solution of saddle point problems.
  Acta Numerica (2005), pp. 1137.







Nonsymmetric saddle-point linear systems

- Nonsymmetric saddle-point linear systems of the form:

$$\begin{bmatrix} \mathbf{M} & \mathbf{A}^\top \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{b} \end{bmatrix},$$

  where $\mathbf{M} \in \mathbb{R}^{m \times m}$ is invertible.
- Monolithic methods: solving the system as a whole, for example, GMRES

  Segregated methods: exploiting the block structure, excluding the preconditioning stage, for example, SPMR, SPQMR, nsLSQR

R. Estrin and C. Greif. *SPMR: A family of saddle-point minimum residual solvers*. SISC, Vol. 40, No. 3 (2018)

K. Du, J.-J. Fan, and F. Wang. *nsLSQR: A quasi-minimum residual method for nonsymmetric saddle-point linear systems*. (2024)

Simultaneous bidiagonalization via $\mathbb{M}$-conjugacy

Algorithm Simultaneous bidiagonalization via $\mathbf{M}$-conjugacy

Require: $\mathbf{M} \in \mathbb{R}^{m\times m}$, $\mathbf{A}$, $\mathbf{B} \in \mathbb{R}^{n\times m}$, and $\mathbf{b}$, $\mathbf{c} \in \mathbb{R}^{n}$

$\beta_1 \mathbf{v}_1 := \mathbf{c},\ \delta_1 \mathbf{z}_1 := \mathbf{b}$

$\mathbf{u} = \mathbf{A}^\top \mathbf{v}_1,\ \mathbf{w} = \mathbf{M}^{-\top}\mathbf{B}^\top \mathbf{z}_1$

$\alpha_1 = |\mathbf{w}^\top \mathbf{u}|^{1/2},\ \gamma_1 = \mathbf{w}^\top \mathbf{u}/\alpha_1$

$\mathbf{u}_1 = \mathbf{M}^{-1}\mathbf{u}/\alpha_1,\ \mathbf{w}_1 = \mathbf{w}/\gamma_1$

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

    $\beta_{k+1}\mathbf{v}_{k+1} := \mathbf{A}\mathbf{w}_k - \alpha_k \mathbf{v}_k,\ \delta_{k+1}\mathbf{z}_{k+1} := \mathbf{B}\mathbf{u}_k - \gamma_k \mathbf{z}_k$

    $\mathbf{u} = \mathbf{A}^\top \mathbf{v}_{k+1} - \beta_{k+1}\mathbf{M}\mathbf{u}_k,\ \mathbf{w} = \mathbf{M}^{-\top}\mathbf{B}^\top \mathbf{z}_{k+1} - \delta_{k+1}\mathbf{w}_k$

    $\alpha_{k+1} = |\mathbf{w}^\top \mathbf{u}|^{1/2},\ \gamma_{k+1} = \mathbf{w}^\top \mathbf{u}/\alpha_{k+1}$

    $\mathbf{u}_{k+1} = \mathbf{M}^{-1}\mathbf{u}/\alpha_{k+1},\ \mathbf{w}_{k+1} = \mathbf{w}/\gamma_{k+1}$

end for

Simultaneous bidiagonalization via $\mathbb{M}$-conjugacy

- Simultaneous bidiagonalization via $\mathbf{M}$-conjugacy:

$$\mathbf{A}\mathbf{W}_k = \mathbf{V}_{k+1}\mathbf{C}_{k+1,k}, \quad \mathbf{A}^\top\mathbf{V}_{k+1} = \mathbf{M}\mathbf{U}_{k+1}\mathbf{C}_{k+1}^\top,$$
$$\mathbf{B}\mathbf{U}_k = \mathbf{Z}_{k+1}\mathbf{F}_{k+1,k}, \quad \mathbf{B}^\top\mathbf{Z}_{k+1} = \mathbf{M}^\top\mathbf{W}_{k+1}\mathbf{F}_{k+1}^\top,$$
$$\mathbf{W}_k^\top\mathbf{M}\mathbf{U}_k = \mathbf{V}_k^\top\mathbf{V}_k = \mathbf{Z}^\top\mathbf{Z}_k = \mathbf{I}_k,$$

where

$$\mathbf{U}_k = \begin{bmatrix}\mathbf{u}_1 & \cdots & \mathbf{u}_k\end{bmatrix}, \quad \mathbf{V}_k = \begin{bmatrix}\mathbf{v}_1 & \cdots & \mathbf{v}_k\end{bmatrix},$$
$$\mathbf{W}_k = \begin{bmatrix}\mathbf{w}_1 & \cdots & \mathbf{w}_k\end{bmatrix}, \quad \mathbf{Z}_k = \begin{bmatrix}\mathbf{z}_1 & \cdots & \mathbf{z}_k\end{bmatrix},$$
$$\mathbf{C}_k = \mathrm{bidiag}(\beta_i, \alpha_i), \quad \mathbf{C}_{k+1,k} = \begin{bmatrix}\mathbf{C}_k \\ \beta_{k+1}\mathbf{e}_k^\top\end{bmatrix},$$
$$\mathbf{F}_k = \mathrm{bidiag}(\delta_i, \gamma_i), \quad \mathbf{F}_{k+1,k} = \begin{bmatrix}\mathbf{F}_k \\ \delta_{k+1}\mathbf{e}_k^\top\end{bmatrix}.$$

SPMR-SC

- The kth SPMR-SC iterate is $\mathbf{x}_k = \mathbf{U}_k \widetilde{\mathbf{x}}_k$, $\mathbf{y}_k = \mathbf{V}_k \widetilde{\mathbf{y}}_k$, where

$$\begin{bmatrix} \widetilde{\mathbf{x}}_k \\ \widetilde{\mathbf{y}}_k \end{bmatrix} = \underset{\widetilde{\mathbf{x}} \in \mathbb{R}^k,\ \widetilde{\mathbf{y}} \in \mathbb{R}^k}{\operatorname{argmin}} \left\| \begin{bmatrix} \mathbf{0} \\ \delta_1 \mathbf{e}_1 \end{bmatrix} - \begin{bmatrix} \mathbf{I}_k & \mathbf{C}_k^\top \\ \mathbf{F}_{k+1,k} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{x}} \\ \widetilde{\mathbf{y}} \end{bmatrix} \right\|_2 .$$

- Equivalent to USYMQR applied to the Schur complement system:

$$-\mathbf{S}\mathbf{y} = \mathbf{b}, \quad \mathbf{S} = \mathbf{B}\mathbf{M}^{-1}\mathbf{A}^\top.$$

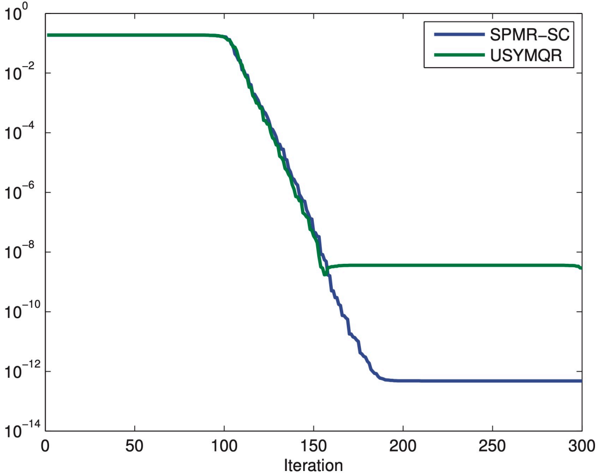
- SPMR-SC can be more numerically stable than USYMQR when the Schur complement is ill-conditioned.

R. Estrin and C. Greif. *SPMR: A family of saddle-point minimum residual solvers.* SISC, Vol. 40, No. 3 (2018)

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)

Example: an ill-conditioned Schur complement

$$\mathrm{cond}(\mathbf{A}) \approx 10^5,\ \mathrm{cond}(\mathbf{B}) \approx 10^5,\ \mathrm{cond}(\mathbf{S}) \approx 10^8$$



Simultaneous bidiagonalization via biorthogonality

Algorithm Simultaneous bidiagonalization via biorthogonality

Require: $\mathbf{M} \in \mathbb{R}^{m \times m}$, $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times m}$, and $\mathbf{b}, \mathbf{c} \in \mathbb{R}^n$

$\delta_1 = |\mathbf{c}^\top \mathbf{b}|^{1/2}, \ \beta_1 = \mathbf{c}^\top \mathbf{b}/\beta_1$

$\mathbf{v}_1 = \mathbf{b}/\delta_1, \ \mathbf{z}_1 = \mathbf{c}/\beta_1$

$\mathbf{u} = \mathbf{A}^\top \mathbf{v}_1, \ \mathbf{w} = \mathbf{M}^{-\top} \mathbf{B}^\top \mathbf{z}_1$

$\alpha_1 = |\mathbf{w}^\top \mathbf{u}|^{1/2}, \ \gamma_1 = \mathbf{w}^\top \mathbf{u}/\alpha_1$

$\mathbf{u}_1 = \mathbf{M}^{-1} \mathbf{u}/\alpha_1, \ \mathbf{w}_1 = \mathbf{w}/\gamma_1$

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

  $\mathbf{v} = \mathbf{B}\mathbf{u}_k - \gamma_k \mathbf{v}_k, \ \mathbf{z} = \mathbf{A}\mathbf{w}_k - \alpha_k \mathbf{z}_k$

  $\delta_{k+1} = |\mathbf{z}^\top \mathbf{v}|^{1/2}, \ \beta_{k+1} = |\mathbf{z}^\top \mathbf{v}|/\delta_{k+1}$

  $\mathbf{v}_{k+1} = \mathbf{v}/\delta_{k+1}, \ \mathbf{z}_{k+1} = \mathbf{z}/\beta_{k+1}$

  $\mathbf{u} = \mathbf{A}^\top \mathbf{v}_{k+1} - \beta_{k+1} \mathbf{M}\mathbf{u}_k, \ \mathbf{w} = \mathbf{M}^{-\top} \mathbf{B}^\top \mathbf{z}_{k+1} - \delta_{k+1} \mathbf{w}_k$

  $\alpha_{k+1} = |\mathbf{w}^\top \mathbf{u}|^{1/2}, \ \gamma_{k+1} = \mathbf{w}^\top \mathbf{u}/\alpha_{k+1}$

  $\mathbf{u}_{k+1} = \mathbf{M}^{-1} \mathbf{u}/\alpha_{k+1}, \ \mathbf{w}_{k+1} = \mathbf{w}/\gamma_{k+1}$

end for

Simultaneous bidiagonalization via biorthogonality

- Simultaneous bidiagonalization via biorthogonality:

$$
\begin{aligned}
&\mathbf{A}\mathbf{W}_k = \mathbf{Z}_{k+1}\mathbf{C}_{k+1,k}, \quad \mathbf{A}^\top \mathbf{V}_{k+1} = \mathbf{M}\mathbf{U}_{k+1}\mathbf{C}_{k+1}^\top, \\
&\mathbf{B}\mathbf{U}_k = \mathbf{V}_{k+1}\mathbf{F}_{k+1,k}, \quad \mathbf{B}^\top \mathbf{Z}_{k+1} = \mathbf{M}^\top \mathbf{U}_{k+1}\mathbf{F}_{k+1}^\top, \\
&\mathbf{W}_k^\top \mathbf{M}\mathbf{U}_k = \mathbf{V}_k^\top \mathbf{Z}_k = \mathbf{I}_k,
\end{aligned}
$$

where

$$
\begin{aligned}
&\mathbf{U}_k = \begin{bmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_k \end{bmatrix}, \quad \mathbf{V}_k = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_k \end{bmatrix}, \\
&\mathbf{W}_k = \begin{bmatrix} \mathbf{w}_1 & \cdots & \mathbf{w}_k \end{bmatrix}, \quad \mathbf{Z}_k = \begin{bmatrix} \mathbf{z}_1 & \cdots & \mathbf{z}_k \end{bmatrix}, \\
&\mathbf{C}_k = \mathrm{bidiag}(\beta_i, \alpha_i), \quad \mathbf{C}_{k+1,k} = \begin{bmatrix} \mathbf{C}_k \\ \beta_{k+1}\mathbf{e}_k^\top \end{bmatrix}, \\
&\mathbf{F}_k = \mathrm{bidiag}(\delta_i, \gamma_i), \quad \mathbf{F}_{k+1,k} = \begin{bmatrix} \mathbf{F}_k \\ \delta_{k+1}\mathbf{e}_k^\top \end{bmatrix}.
\end{aligned}
$$

SPQMR-SC

- The kth SPQMR-SC iterate is $\mathbf{x}_k = \mathbf{U}_k \widetilde{\mathbf{x}}_k$, $\mathbf{y}_k = \mathbf{V}_k \widetilde{\mathbf{y}}_k$, where

$$\begin{bmatrix} \widetilde{\mathbf{x}}_k \\ \widetilde{\mathbf{y}}_k \end{bmatrix} = \underset{\widetilde{\mathbf{x}} \in \mathbb{R}^k,\ \widetilde{\mathbf{y}} \in \mathbb{R}^k}{\operatorname{argmin}} \left\| \begin{bmatrix} \mathbf{0} \\ \delta_1 \mathbf{e}_1 \end{bmatrix} - \begin{bmatrix} \mathbf{I}_k & \mathbf{C}_k^\top \\ \mathbf{F}_{k+1,k} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{x}} \\ \widetilde{\mathbf{y}} \end{bmatrix} \right\|_2 .$$

- Equivalent to QMR applied to the Schur complement system:

$$-\mathbf{S}\mathbf{y} = \mathbf{b}, \quad \mathbf{S} = \mathbf{B}\mathbf{M}^{-1}\mathbf{A}^\top.$$

- The convergence of SPMR-SC is monotonic, while the convergence of SPQMR-SC is erratic.

R. Estrin and C. Greif. *SPMR: A family of saddle-point minimum residual solvers.* SISC, Vol. 40, No. 3 (2018)

R. W. Freund and N. M. Nachtigal. *QMR: A Quasi-Minimal Residual Method for Non-Hermitian Linear-Systems.* NM, Vol. 60, Iss. 3 (1991)

Bidiagonal-Hessenberg reduction

Algorithm Bidiagonal-Hessenberg reduction

Require: $\mathbf{M} \in \mathbb{R}^{m\times m}$, $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n\times m}$, $\mathbf{b} \in \mathbb{R}^n$

$\mathbf{u}_1 = \mathbf{b}/\beta_1$ with $\beta_1 = \|\mathbf{b}\|_2$

$\mathbf{v} = \mathbf{A}^\top \mathbf{u}_1$, $\mathbf{v}_1 = \mathbf{M}^{-1}\mathbf{v}$, $\alpha_1 = \begin{cases} |\mathbf{v}_1^\top \mathbf{v}|^{1/2} & \text{if} \quad \mathbf{v}_1^\top \mathbf{v} \neq 0 \\ \|\mathbf{v}_1\|_2 & \text{if} \quad \mathbf{v}_1^\top \mathbf{v} = 0 \end{cases}$

$\mathbf{v}_1 = \mathbf{v}_1/\alpha_1$

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

    $\mathbf{u} = \mathbf{B}\mathbf{v}_k$

    for $i = 1, 2, \ldots, k$ **do**

        $h_{ik} = \mathbf{u}_i^\top \mathbf{u}$

        $\mathbf{u} = \mathbf{u} - h_{ik}\mathbf{u}_i$

    end for

    $\mathbf{u}_{k+1} = \mathbf{u}/\beta_{k+1}$ with $\beta_{k+1} = \|\mathbf{u}\|_2$

    $\mathbf{v} = \mathbf{A}^\top \mathbf{u}_{k+1} - \beta_{k+1}\mathbf{M}\mathbf{v}_k$, $\mathbf{v}_{k+1} = \mathbf{M}^{-1}\mathbf{v}$, $\alpha_{k+1} = \begin{cases} |\mathbf{v}_{k+1}^\top \mathbf{v}|^{1/2} & \text{if} \quad \mathbf{v}_{k+1}^\top \mathbf{v} \neq 0 \\ \|\mathbf{v}_{k+1}\|_2 & \text{if} \quad \mathbf{v}_{k+1}^\top \mathbf{v} = 0 \end{cases}$

    $\mathbf{v}_{k+1} = \mathbf{v}_{k+1}/\alpha_{k+1}$

end for

Bidiagonal-Hessenberg reduction

- Bidiagonal-Hessenberg reduction:

$$\mathbf{A}^\top \mathbf{U}_k = \mathbf{M}\mathbf{V}_k \mathbf{C}_k^\top, \qquad \mathbf{U}_{k+1}^\top \mathbf{U}_{k+1} = \mathbf{I}_{k+1},$$
$$\mathbf{B}\mathbf{V}_k = \mathbf{U}_{k+1}\mathbf{H}_{k+1,k} = \mathbf{U}_k \mathbf{H}_k + \beta_{k+1}\mathbf{u}_{k+1}\mathbf{e}_k^\top,$$

where

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

$$\mathbf{C}_k = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \end{bmatrix}, \; \mathbf{H}_{k+1,k} = \begin{bmatrix} h_{11} & \cdots & h_{1k} \\ h_{21} & \ddots & \vdots \\ & \ddots & h_{kk} \\ & & h_{k+1,k} \end{bmatrix}.$$

nsLSQR

- The kth nsLSQR iterate is $\mathbf{x}_k = \mathbf{V}_k \widetilde{\mathbf{x}}_k$, $\mathbf{y}_k = \mathbf{U}_k \widetilde{\mathbf{y}}_k$, where

$$\begin{bmatrix} \widetilde{\mathbf{x}}_k \\ \widetilde{\mathbf{y}}_k \end{bmatrix} = \underset{\widetilde{\mathbf{x}} \in \mathbb{R}^k,\ \widetilde{\mathbf{y}} \in \mathbb{R}^k}{\operatorname{argmin}} \left\| \begin{bmatrix} \mathbf{0} \\ \beta_1 \mathbf{e}_1 \end{bmatrix} - \begin{bmatrix} \mathbf{I}_k & \mathbf{C}_k^\top \\ \mathbf{H}_{k+1,k} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{x}} \\ \widetilde{\mathbf{y}} \end{bmatrix} \right\|_2 .$$

- Equivalent to GMRES applied to the Schur complement system:

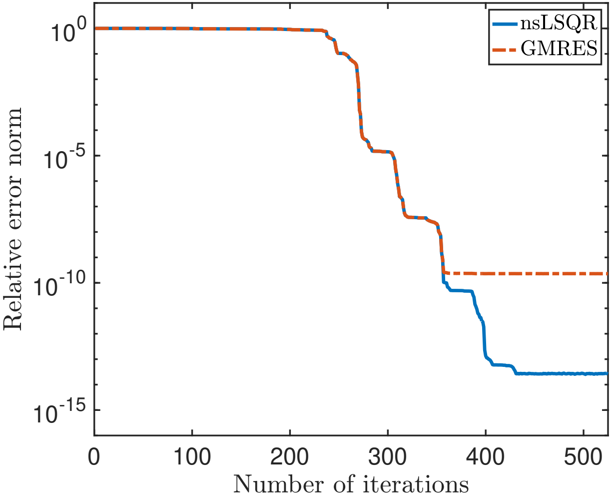
$$-\mathbf{S}\mathbf{y} = \mathbf{b}, \quad \mathbf{S} = \mathbf{B}\mathbf{M}^{-1}\mathbf{A}^\top.$$

- nsLSQR can be more numerically stable than GMRES when the Schur complement is ill-conditioned.

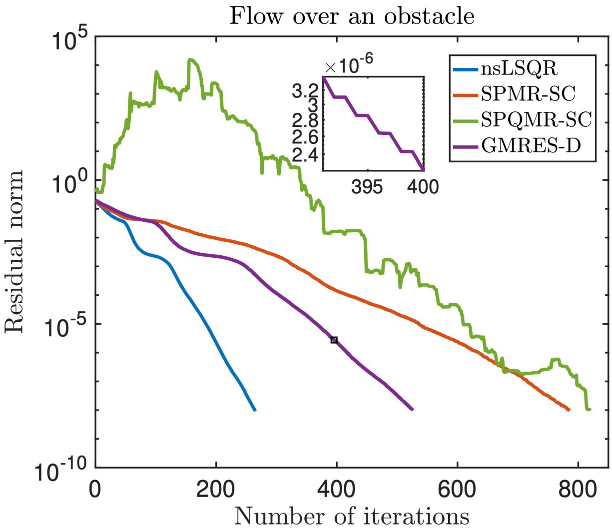
K. Du, J.-J. Fan, and F. Wang. *nsLSQR: A quasi-minimum residual method for nonsymmetric saddle-point linear systems.* (2024)

Example: an ill-conditioned Schur complement

$$\mathrm{cond}(\mathbf{A}) \approx 7 \times 10^3,\ \mathrm{cond}(\mathbf{B}) \approx 7 \times 10^3,\ \mathrm{cond}(\mathbf{S}) \approx 5 \times 10^7$$



Example: Flow over an obstacle (IFISS)



Nonsymmetric partitioned linear systems

- Nonsymmetric partitioned linear systems of the form

$$\begin{bmatrix} \lambda \mathbf{I} & \mathbf{A} \\ \mathbf{B} & \mu \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}.$$

  Note that λ and/or μ may be zero.
- Monolithic methods: solving the system as a whole, for example, GMRES

  Segregated methods: exploiting the block structure, excluding the preconditioning stage, for example, GPMR, GPBiLQ, GPQMR

A. Montoison and D. Orban. *GPMR: An iterative method for unsymmetric partitioned linear systems*. SIMAX, Vol. 44, No. 1 (2023)

K. Du, J.-J. Fan, and F. Wang. *GPBiLQ and GPQMR: Two iterative methods for unsymmetric partitioned linear systems*. arXiv:2401.02608 (2024)

Simultaneous orthogonal Hessenberg reduction

Algorithm Simultaneous orthogonal Hessenberg reduction

Require: $\mathbf{A}$, $\mathbf{B}$, $\mathbf{b}$, $\mathbf{c}$, all nonzero

$\beta \mathbf{v}_1 := \mathbf{b}$, $\gamma \mathbf{u}_1 := \mathbf{c}$

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

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

        $h_{ik} = \mathbf{v}_i^\top \mathbf{A} \mathbf{u}_k$

        $f_{ik} = \mathbf{u}_i^\top \mathbf{B} \mathbf{v}_k$

    end for

    $h_{k+1,k} \mathbf{v}_{k+1} = \mathbf{A} \mathbf{u}_k - \sum_{i=1}^{k} h_{ik} \mathbf{v}_i$

    $f_{k+1,k} \mathbf{u}_{k+1} = \mathbf{B} \mathbf{v}_k - \sum_{i=1}^{k} f_{ik} \mathbf{u}_i$

end for

Simultaneous orthogonal Hessenberg reduction

- Simultaneous orthogonal Hessenberg reduction

$$
\begin{aligned}
\mathbf{A}\mathbf{U}_k &= \mathbf{V}_k\mathbf{H}_k + h_{k+1,k}\mathbf{v}_{k+1}\mathbf{e}_k^\top = \mathbf{V}_{k+1}\mathbf{H}_{k+1,k},\\
\mathbf{B}\mathbf{V}_k &= \mathbf{U}_k\mathbf{F}_k + f_{k+1,k}\mathbf{u}_{k+1}\mathbf{e}_k^\top = \mathbf{U}_{k+1}\mathbf{F}_{k+1,k},\\
\mathbf{V}_{k+1}^\top\mathbf{V}_{k+1} &= \mathbf{U}_{k+1}^\top\mathbf{U}_{k+1} = \mathbf{I}_{k+1},
\end{aligned}
$$

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

$$
\mathbf{H}_{k+1,k} = \begin{bmatrix} h_{11} & \cdots & h_{1k} \\ h_{21} & \ddots & \vdots \\ & \ddots & h_{kk} \\ & & h_{k+1,k} \end{bmatrix}, \mathbf{F}_{k+1,k} = \begin{bmatrix} f_{11} & \cdots & f_{1k} \\ f_{21} & \ddots & \vdots \\ & \ddots & f_{kk} \\ & & f_{k+1,k} \end{bmatrix}.
$$

GPMR

- The kth GPMR iterate is

$$\begin{bmatrix}\mathbf{x}_k\\ \mathbf{y}_k\end{bmatrix} = \underset{\mathbf{x}\in\text{range}(\mathbf{V}_k),\ \mathbf{y}\in\text{range}(\mathbf{U}_k)}{\text{argmin}} \left\| \begin{bmatrix}\mathbf{b}\\ \mathbf{c}\end{bmatrix} - \begin{bmatrix}\lambda\mathbf{I} & \mathbf{A}\\ \mathbf{B} & \mu\mathbf{I}\end{bmatrix} \begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix} \right\|_2.$$

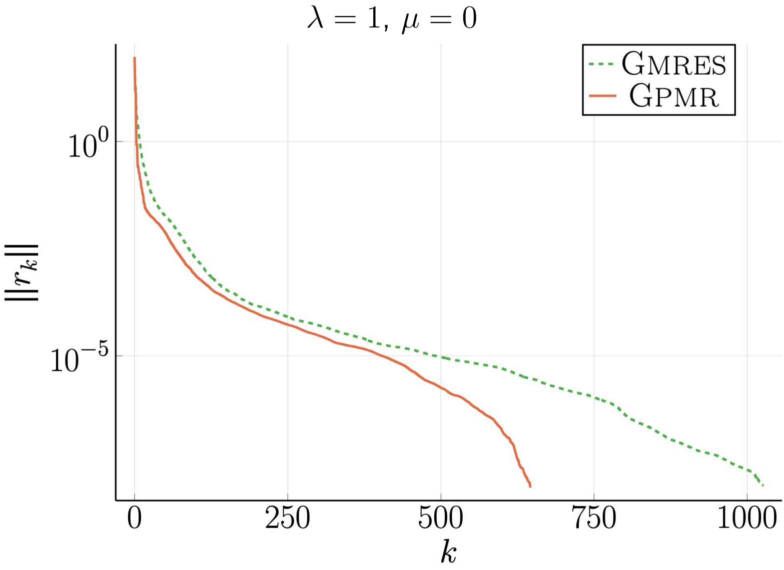
- Equivalent to Block-GMRES:

$$\begin{bmatrix}\lambda\mathbf{I} & \mathbf{A}\\ \mathbf{B} & \mu\mathbf{I}\end{bmatrix} \begin{bmatrix}\mathbf{x}^1 & \mathbf{x}^2\\ \mathbf{y}^1 & \mathbf{y}^2\end{bmatrix} = \begin{bmatrix}\mathbf{b} & \mathbf{0}\\ \mathbf{0} & \mathbf{c}\end{bmatrix}.$$

- GPMR terminates significantly earlier than GMRES on a residual-based stopping criterion with an improvement up to 50% in terms of number of iterations.

A. Montoison and D. Orban. *GPMR: An iterative method for unsymmetric partitioned linear systems*. SIMAX, Vol. 44, No. 1 (2023)

Example: $\mathbf{A} =$ `well1850`, $\mathbf{B} =$ `illc1850`



Randomized Numerical Linear Algebra +

- Arguably, the most exciting recent development in NLA is the advent of new randomized algorithms that are fast, scalable, robust, and reliable.
- Intelligent solvers.

M. Dereziński, Michael W. Mahoney. *Recent and Upcoming Developments in Randomized Numerical Linear Algebra for Machine Learning*. arXiv:2406.11151 (2024)

A. Kireeva and J. A. Tropp. *Randomized matrix computations: Themes and variations*. arXiv:2402.17873 (2024)

J. A. Tropp and R. J. Webber. *Randomized algorithms for low-rank matrix approximation: Design, analysis, and applications*. arXiv:2306.12418 (2023)

R. Murray et al. *Randomized Numerical Linear Algebra : A perspective on the field with an eye to software*, arXiv:2302.11474 (2023)

Haifeng Zou, Xiaowen Xu, Chen-Song Zhang. *A Survey on Intelligent Iterative Methods for Solving Sparse Linear Algebraic Equations.* arXiv:2310.06630 (2023)

Randomized Gram–Schmidt process

Algorithm 2.1. RGS algorithm

Given: $n \times m$ matrix $\mathbf{W}$ and $k \times n$ matrix $\mathbf{\Theta}$, $m \le k \ll n$.
Output: $n \times m$ factor $\mathbf{Q}$ and $m \times m$ upper triangular factor $\mathbf{R}$.
for $i = 1 : m$ **do**

1. Sketch $\mathbf{w}_i$: $\mathbf{p}_i = \mathbf{\Theta}\mathbf{w}_i$. # macheps: u_{fine}
2. Solve $k \times (i-1)$ least-squares problem:
   $[\mathbf{R}]_{(1:i-1,i)} = \arg\min_{\mathbf{y}} \|\mathbf{S}_{i-1}\mathbf{y} - \mathbf{p}_i\|$. # macheps: u_{fine}
3. Compute projection of $\mathbf{w}_i$: $\mathbf{q}'_i = \mathbf{w}_i - \mathbf{Q}_{i-1}[\mathbf{R}]_{(1:i-1,i)}$. # macheps: u_{crs}
4. Sketch $\mathbf{q}'_i$: $\mathbf{s}'_i = \mathbf{\Theta}\mathbf{q}'_i$. # macheps: u_{fine}
5. Compute the sketched norm $r_{i,i} = \|\mathbf{s}'_i\|$. # macheps: u_{fine}
6. Scale vector $\mathbf{s}_i = \mathbf{s}'_i / r_{i,i}$. # macheps: u_{fine}
7. Scale vector $\mathbf{q}_i = \mathbf{q}'_i / r_{i,i}$. # macheps: u_{fine}

end for

8. (Optional) compute $\Delta_m = \|\mathbf{I}_{m\times m} - \mathbf{S}_m^{\mathrm{T}}\mathbf{S}_m\|_{\mathrm{F}}$ and $\tilde{\Delta}_m = \frac{\|\mathbf{P}_m - \mathbf{S}_m\mathbf{R}_m\|_{\mathrm{F}}}{\|\mathbf{P}_m\|_{\mathrm{F}}}$.
   Use Theorem 3.2 to certify the output. # macheps: u_{fine}

$\mathbf{W} = \mathbf{QR}$, $\mathbf{\Theta W} = \mathbf{\Theta QR}$, $(\mathbf{\Theta Q})^\top(\mathbf{\Theta Q}) = \mathbf{I}_m$, $\mathrm{cond}(\mathbf{Q})$ is small

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Randomized GMRES (rGMRES) for $\mathrm{Ax} = \mathrm{b}$

Algorithm 4.1. RGS-Arnoldi algorithm

Given: $n \times n$ matrix $\mathbf{A}$, $n \times 1$ vector $\mathbf{b}$, $k \times n$ matrix $\mathbf{\Theta}$ with $k \ll n$, parameter m.
Output: $n \times m$ factor $\mathbf{Q}_m$ and $m \times m$ upper triangular factor $\mathbf{R}_m$.
1. Set $\mathbf{w}_1 = \mathbf{b}$.
2. Perform 1st iteration of Algorithm 2.1.

for $i = 2 : m$ **do**
   3. Compute $\mathbf{w}_i = \mathbf{A}\mathbf{q}_{i-1}$. # macheps: u_{fine}
   4. Perform ith iteration of Algorithm 2.1.

end for
5. (Optional) Compute Δ_m and $\tilde{\Delta}_m$.
   Use Proposition 4.1 to certify the output. # macheps: u_{fine}

- $(\mathbf{\Theta}\mathbf{Q}_m)^\top(\mathbf{\Theta}\mathbf{Q}_m) = \mathbf{I}_m$ and $\mathbf{Q}_m$ is nonorthogonal.
- rGMRES: $\mathbf{x}_m = \mathbf{Q}_m\mathbf{y}_m$, where $\mathbf{y}_m$ solves

$$\min_{\mathbf{y}} \|\mathbf{H}_{m+1,m}\mathbf{y} - r_{11}\mathbf{e}_1\|_2.$$

- $\|\mathbf{r}^{\mathrm{GMRES}}\|_2 \le \|\mathbf{r}^{\mathrm{rGMRES}}\|_2 \le \mathrm{const} \cdot \|\mathbf{r}^{\mathrm{GMRES}}\|_2 \quad \mathrm{whp}.$

Sketched GMRES (sGMRES) for $\mathbf{Ax} = \mathbf{b}$

- Columns of $\mathbf{B}$ form a basis of the Krylov subspace $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$.
- GMRES: $\mathbf{x_B} = \mathbf{B}\mathbf{y}_\star$, where Arnoldi process is used for $\mathbf{B}$ and $\mathbf{y}_\star$ solves the overdetermined least-squares problem

$$\min_{\mathbf{y}} \|\mathbf{ABy} - \mathbf{b}\|_2.$$

- sGMRES uses "skecth-and-solve" and is faster: $\widehat{\mathbf{x}} = \mathbf{B}\widehat{\mathbf{y}}$, where $\mathbf{B}$ can be a nonorthogonal basis (for example, using k-truncated Arnoldi) and $\widehat{\mathbf{y}}$ solves the sketched problem

$$\min_{\mathbf{y}} \|\mathbf{S}(\mathbf{ABy} - \mathbf{b})\|_2.$$

- $\|\mathbf{r}^{\mathrm{GMRES}}\|_2 \le \|\mathbf{r}^{\mathrm{sGMRES}}\|_2 \le \mathrm{const} \cdot \|\mathbf{r}^{\mathrm{GMRES}}\|_2 \quad \mathrm{whp.}$

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sGMRES + k-truncated Arnoldi

Algorithm 1.1. sGMRES + k-truncated Arnoldi.

Input: Matrix $\boldsymbol{A} \in \mathbb{C}^{n \times n}$, right-hand side $\boldsymbol{f} \in \mathbb{C}^n$, initial guess $\boldsymbol{x} \in \mathbb{C}^n$, basis dimension d, number k of vectors for truncated orthogonalization, stability tolerance $\texttt{tol} = O(u^{-1})$.

Output: Approximate solution $\hat{\boldsymbol{x}} \in \mathbb{C}^n$ to linear system (1.5) and estimated residual norm $\hat{r}_{\text{est}}$

1 **function sGMRES**
2 Draw subspace embedding $\boldsymbol{S} \in \mathbb{C}^{s \times n}$ with $s = 2(d+1)$ ▷ See subsection 2.4
3 Form residual and sketch: $\boldsymbol{r} = \boldsymbol{f} - \boldsymbol{A}\boldsymbol{x}$ and $\boldsymbol{g} = \boldsymbol{S}\boldsymbol{r}$
4 Normalize basis vector $\boldsymbol{b}_1 = \boldsymbol{r}/\|\boldsymbol{r}\|_2$ and apply matrix $\boldsymbol{m}_1 = \boldsymbol{A}\boldsymbol{b}_1$
5 **for** $j = 2, 3, 4, \ldots, d$ **do** ▷ See also subsection 5.2
6 Truncated Arnoldi: $\boldsymbol{w}_j = (\mathbf{I} - \boldsymbol{b}_{j-1}\boldsymbol{b}_{j-1}^* - \ldots - \boldsymbol{b}_{j-k}\boldsymbol{b}_{j-k}^*)\boldsymbol{m}_{j-1}$ ▷ $\boldsymbol{b}_{-i} = \mathbf{0}$ for $i \geq 0$
7 Normalize basis vector $\boldsymbol{b}_j = \boldsymbol{w}_j/\|\boldsymbol{w}_j\|_2$ and apply matrix $\boldsymbol{m}_j = \boldsymbol{A}\boldsymbol{b}_j$
8 Sketch reduced matrix: $\boldsymbol{C} = \boldsymbol{S}[\boldsymbol{m}_1, \ldots, \boldsymbol{m}_d]$
9 Thin QR factorization: $\boldsymbol{C} = \boldsymbol{U}\boldsymbol{T}$
10 **if** condition number $\kappa_2(\boldsymbol{T}) > \texttt{tol}$ **then** warning...
11 Either whiten $\boldsymbol{B} \leftarrow \boldsymbol{B}\boldsymbol{T}^{-1}$ or form new residual and restart ▷ See subsection 5.3
12 Solve least-squares problem: $\hat{\boldsymbol{y}} = \boldsymbol{T}^{-1}(\boldsymbol{U}^*\boldsymbol{g})$ ▷ See (3.7)
13 Residual estimate: $\hat{r}_{\text{est}} = \|(\mathbf{I} - \boldsymbol{U}\boldsymbol{U}^*)\boldsymbol{g}\|_2$ ▷ See (3.8)
14 Construct solution: $\hat{\boldsymbol{x}} = \boldsymbol{x} + [\ \boldsymbol{b}_1, \ldots,\ \boldsymbol{b}_d]\hat{\boldsymbol{y}}$

Implementation: In line 6, use double Gram–Schmidt for stability. In line 9, the QR factorization may require pivoting. In lines 11–12, apply $\boldsymbol{T}^{-1}$ via triangular substitution.

rGMRES vs sGMRES

- rGMRES uses sketching to reduce the orthogonalization cost.
- sGMRES uses "sketch-and-solve" to reduce computational cost, is asymptotically faster, and has more flexibility.

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Summary

- We have presented nsLSQR for nonsymmetric saddle-point linear systems.
- nsLSQR is mathematically equivalent to GMRES applied to the corresponding Schur complement system, but may be numerically superior.
- nsLSQR usually is faster than SPMR-SC and SPQMR-SC in terms of the number of iterations, and if the iteration cost is dominated by the $\mathbf{M}$-solve rather than reorthogonalization, then nsLSQR should be the preferred method.
- The ideas of rGMRES and sGMRES can be used for GPMR and nsLSQR.
- Intelligent iterative methods for block two-by-two linear systems?

Thanks!