Numerical behavior of GMRES for singular EP and GP systems

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Generalized Minimal RESidual method [Saad, Schultz 1986]

Given the system $A\boldsymbol{x} = \boldsymbol{b}$, the initial guess $\boldsymbol{x}_0$ and residual $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$, GMRES computes $\boldsymbol{x}_k$ over $\boldsymbol{x}_0 + \mathcal{K}_k(A, \boldsymbol{r}_0)$, where

$$\mathcal{K}_k(A, \boldsymbol{r}_0) = \operatorname{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{k-1}\boldsymbol{r}_0\}$$

is the k-th Krylov subspace, such that $\boldsymbol{x}_k$ minimizes $\|\boldsymbol{b} - A\boldsymbol{x}_k\|$.

Let $AQ_k = Q_{k+1}H_{k+1,k}$ be the Arnoldi decomposition, where the columns of $Q_k \in \mathbb{R}^{n\times k}$ form an orthonormal basis of $\mathcal{K}_k$ and $H_{k+1,k} \in \mathbb{R}^{(k+1)\times k}$ is an extended Hessenberg matrix.

Then the iterate $\boldsymbol{x}_k = \boldsymbol{x}_0 + Q_k\boldsymbol{y}_k$ satisfies

$$\begin{aligned}\|\boldsymbol{b} - A\boldsymbol{x}_k\| &= \|\boldsymbol{r}_0 - AQ_k\boldsymbol{y}_k\| = \|\,\|\boldsymbol{r}_0\|\boldsymbol{e}_1 - H_{k+1,k}\boldsymbol{y}_k\| \\ &= \min_{\boldsymbol{y}\in\mathbb{R}^k} \|\,\|\boldsymbol{r}_0\|\boldsymbol{e}_1 - H_{k+1,k}\boldsymbol{y}\|, \quad \boldsymbol{e}_1 = [1, 0, \ldots, 0]^{\mathsf{T}}.\end{aligned}$$

Numerical behavior of GMRES

The restriction $A|_{\mathcal{K}_k}$ of A to the Krylov subspace $\mathcal{K}_k \subseteq \mathbb{R}^n$ plays an important role. Its condition number is defined as

$$\kappa(A|_{\mathcal{K}_k}) = \frac{\max_{z\in\mathcal{K}_k\setminus\{\mathbf{0}\}} ||Az|| \Big/ ||z||}{\min_{z\in\mathcal{K}_k\setminus\{\mathbf{0}\}} ||Az|| \Big/ ||z||}.$$

The identity $\kappa(A|_{\mathcal{K}_k}) = \kappa(H_{k+1,k})$ ($\equiv ||H_{k+1,k}||||H^{\dagger}_{k+1,k}||$) follows from

$$\{\max,\min\}_{z\in\mathcal{K}_k\setminus\{\mathbf{0}\}}\frac{||Az||}{||z||} = \{\max,\min\}_{\boldsymbol{w}\in\mathbb{R}^k\setminus\{\mathbf{0}\}}\frac{||AQ_k\boldsymbol{w}||}{||Q_k\boldsymbol{w}||} = \{\max,\min\}_{\boldsymbol{w}\in\mathbb{R}^k\setminus\{\mathbf{0}\}}\frac{||H_{k+1,k}\boldsymbol{w}||}{||\boldsymbol{w}||}.$$

The accuracy of $\boldsymbol{x}_k$ computed in finite precision arithmetic is affected by the conditioning of $H_{k+1,k}$.

GMRES applied to nonsingular systems

¿From $AQ_k = Q_{k+1}H_{k+1,k}$ and $Q_{k+1}^T Q_{k+1} = I_{k+1}$ it follows that

$$\|H_{k+1,k}\| = \|AQ_k\| \leq \|A\|\|Q_k\| = \|A\|$$

and for nonsingular A we have

$$\sigma_k(H_{k+1,k}) = \sigma_k(AQ_k) \geq \sigma_n(A)\sigma_k(Q_k) \geq \sigma_n(A) > 0.$$

Then the solution $\boldsymbol{y}_k = H_{k+1,k}^{\dagger}\|\boldsymbol{r}_0\|\boldsymbol{e}_1$ of the upper Hessenberg least squares problem satisfies the bounds

$$\|\boldsymbol{y}_k\| \leq \frac{\|\boldsymbol{r}_0\|}{\sigma_k(H_{k+1,k})} \leq \frac{\|\boldsymbol{r}_0\|}{\sigma_n(A)}.$$

GMRES on singular systems - example of a breakdown

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \in \mathcal{R}(A),$$

$$\mathcal{R}(A) = \mathcal{N}(A) = \operatorname{span}\left\{\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right\}, \quad \mathcal{R}(A^{\mathsf{T}}) = \mathcal{N}(A^{\mathsf{T}}) = \operatorname{span}\left\{\begin{bmatrix} 0 \\ 1 \end{bmatrix}\right\},$$

$$\boldsymbol{x}_0 = 0, \quad \boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0 \in \mathcal{N}(A)$$

If $\boldsymbol{b} \in \mathcal{R}(A)$ and $\boldsymbol{r}_0 \in \mathcal{R}(A) \cap \mathcal{N}(A) \neq \{\mathbf{0}\}$, then GMRES breaks down at step 1 without determining a solution of $A\boldsymbol{x} = \boldsymbol{b}$.

Range-symmetric (EP) systems

A matrix $A \in \mathbb{R}^{n\times n}$ s.t. $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A)$, is called an EP (equal projection) or range-symmetric matrix.

Theorem ([Brown, Walker, SIMAX 97])

If $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A)$, then GMRES gives a solution $\boldsymbol{x}_*$ of $\min_{\boldsymbol{x}\in\mathbb{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|$ without breakdown for all $\boldsymbol{b} \in \mathbb{R}^n$ and $\forall \boldsymbol{x}_0 \in \mathbb{R}^n$.

Note that $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A) \Longrightarrow \mathcal{N}(A) \cap \mathcal{R}(A) = \{\mathbf{0}\}$.

We say a matrix A such that $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\mathbf{0}\}$ is a group (GP) matrix.

Range-symmetric (EP) system, consistent case $\boldsymbol{b} \in \mathcal{R}(A)$

Since $\mathcal{K}_k \subseteq \mathcal{R}(A)$, we have

$$\sigma_k(H_{k+1,k}) = \min_{z \in \mathcal{K}_k \setminus \{\mathbf{0}\}} \frac{||Az||}{||z||} \geq \min_{z \in \mathcal{R}(A) \setminus \{\mathbf{0}\}} \frac{||Az||}{||z||}$$

and thus $\kappa(H_{k+1,k}) \leq \kappa(A|_{\mathcal{R}(A)})$. If A is EP, then

$$\min_{z \in \mathcal{R}(A) \setminus \{\mathbf{0}\}} \frac{||Az||}{||z||} = \min_{z \in \mathcal{R}(A^{\mathsf{T}}) \setminus \{\mathbf{0}\}} \frac{||Az||}{||z||} = \sigma_{min}(A) > 0$$

and

$$\kappa(A|_{\mathcal{R}(A)}) = \frac{||A||}{\min_{z \in \mathcal{R}(A^{\mathsf{T}}) \setminus \{\mathbf{0}\}} ||Az||/||z||} = \kappa(A).$$

Consistent EP case $\sim$ nonsingular case, i.e., $\kappa(H_{k+1,k}) \leq \kappa(A)$.

Range-symmetric (EP) system, inconsistent case $\boldsymbol{b} \notin \mathcal{R}(A)$

Since $\mathcal{R}(A^{\mathsf{T}}) = \mathcal{R}(A) \Longleftrightarrow \mathcal{N}(A^T) = \mathcal{N}(A)$, the LS residual $\boldsymbol{r}_* = \boldsymbol{b}|_{\mathcal{N}(A^T)}$ satisfies $A^{\mathsf{T}}\boldsymbol{r}_* = 0$, and so $\boldsymbol{r}_* \in \mathcal{N}(A^{\mathsf{T}})$ belongs also to $\mathcal{N}(A)$ with

$$\sigma_k(H_{k+1,k}) = \min_{z \in \mathcal{K}_k \setminus \{\mathbf{0}\}} \frac{\|Az\|}{\|z\|} \geq \min_{z \in \mathrm{span}\{\boldsymbol{r}_*\} \cup \mathcal{R}(A) \setminus \{\mathbf{0}\}} \frac{\|Az\|}{\|z\|} = 0.$$

Since $\boldsymbol{r}_{k-1} \in \mathcal{K}_k$ satisfies $\boldsymbol{r}_{k-1} - \boldsymbol{r}_* \in \mathcal{R}(A)$ and $A\boldsymbol{r}_* = \mathbf{0}$, we have

$$\sigma_k(H_{k+1,k}) = \min_{z \in \mathcal{K}_k \setminus \{\mathbf{0}\}} \frac{\|Az\|}{\|z\|} \leq \frac{\|A\boldsymbol{r}_{k-1}\|}{\|\boldsymbol{r}_{k-1}\|} = \frac{\|A(\boldsymbol{r}_{k-1} - \boldsymbol{r}_*)\|}{\|\boldsymbol{r}_{k-1}\|} \leq \|A\| \frac{\|\boldsymbol{r}_{k-1} - \boldsymbol{r}_*\|}{\|\boldsymbol{r}_{k-1}\|}.$$

The Hessenberg least squares problem thus becomes very ill-conditioned before a LS solution is reached by GMRES.

EP case for $\boldsymbol{b} \notin \mathcal{R}(A)$

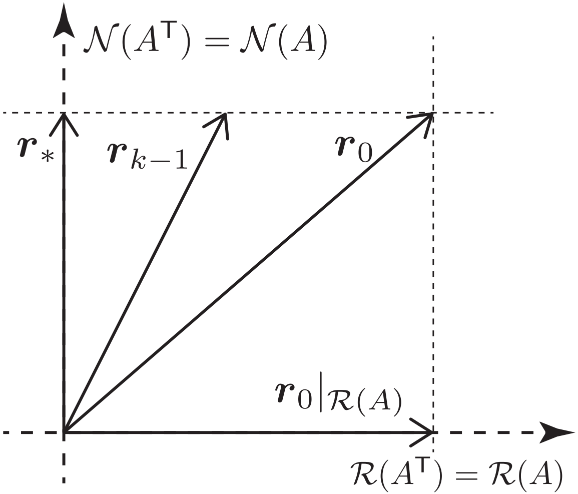


Figure: Geometric illustration of residual vectors.

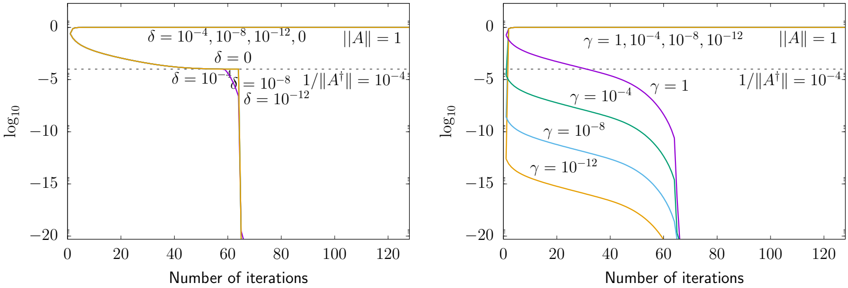
Example: small singular EP system

$$A = \begin{bmatrix} \mathrm{diag}(10^{\frac{0}{127}}, 10^{\frac{-4}{127}}, 10^{\frac{-8}{127}}, \ldots, 10^{-4}) & \mathrm{O} \\ \mathrm{O} & \mathrm{O} \end{bmatrix} \in \mathbb{R}^{128\times 128}, \quad \boldsymbol{b} = \begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\delta} \end{bmatrix},$$

where $\boldsymbol{\gamma} = [\gamma, \ldots, \gamma]^{\mathsf{T}} \in \mathbb{R}^{64}$ and $\boldsymbol{\delta} = [\delta, \ldots, \delta]^{\mathsf{T}} \in \mathbb{R}^{64}$, i.e., $\kappa(A) = 10^4$, and $\boldsymbol{b} \notin \mathcal{R}(A) \iff \delta \neq 0$.

Inconsistency is controlled by δ/γ.

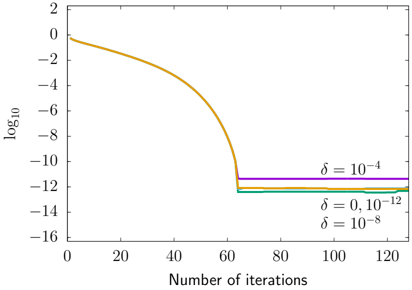
Example: GMRES

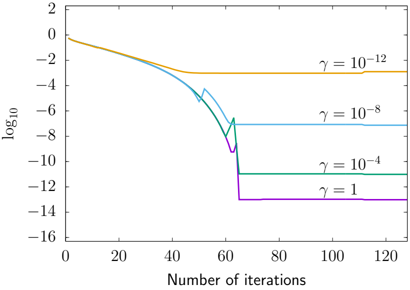


(a) Weakly inconsistent cases $\gamma = 1$. (b) Strongly inconsistent cases $\delta = 1$.

Figure: Extreme singular values of A and $H_{k+1,k}$.

Example: GMRES





(a) Weakly inconsistent cases $\gamma = 1$. (b) Strongly inconsistent cases $\delta = 1$.

Figure: Relative residual norm $\|A^{\mathsf{T}}\boldsymbol{r}_k\|/\|A^{\mathsf{T}}\boldsymbol{b}\|$.

Singular value decomposition of A

$$A = U\Sigma V^{\mathsf{T}} = [U_1, U_2] \begin{bmatrix} \Sigma_1 & \mathrm{O} \\ \mathrm{O} & \mathrm{O} \end{bmatrix} [V_1, V_2]^T,$$

where Σ_1 is diagonal with positive singular values, $U = [U_1, U_2]$ and $V = [V_1, V_2]$ are orthogonal matrices,

$$\mathcal{R}(A) = \mathcal{R}(U_1), \qquad \mathcal{R}(A)^{\perp} = \mathcal{N}(A^{\mathsf{T}}) = \mathcal{R}(U_2),$$
$$\mathcal{N}(A)^{\perp} = \mathcal{R}(A^{\mathsf{T}}) = \mathcal{R}(V_1), \qquad \mathcal{N}(A) = \mathcal{R}(V_2),$$

EP and GP matrices via singular value decomposition

- An EP matrix A, $\mathcal{R}(A^{\mathsf{T}}) = \mathcal{R}(A)$, satisfies

$$\mathcal{R}(V_1) = \mathcal{R}(U_1) \quad \Longleftrightarrow \quad V_1^{\mathsf{T}} U_1 \text{ is orthogonal}$$

  since $V_1^{\mathsf{T}} U_2 = \mathrm{O}$.
- A GP matrix A, $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\mathbf{0}\}$, satisfies

$$\mathcal{R}(U_1) \cap \mathcal{R}(V_2) = \{\mathbf{0}\} \Longleftrightarrow \mathrm{rank}([U_1, V_2]) = n \Longleftrightarrow V_1^{\mathsf{T}} U_1 \text{ is nonsingular,}$$

  but $V_1^{\mathsf{T}} U_1$ can be ill-conditioned.

The cosines of the principal angles between $\mathcal{R}(A)$ and $\mathcal{R}(A^{\mathsf{T}})$ are the singular values of $V_1^{\mathsf{T}} U_1$.

- EP: Cosines between $\mathcal{R}(A)$ and $\mathcal{R}(A^{\mathsf{T}})$ are all zero
- GP: Condition number of $V_1^{\mathsf{T}} U_1$ are the ratio of the cosines

Group inverse and Moore-Penrose inverse of A

$$A^\dagger = [V_1, V_2] \begin{bmatrix} \Sigma_1^{-1} & \mathrm{O} \\ \mathrm{O} & \mathrm{O} \end{bmatrix} [U_1, U_2]^T$$

$$\mathcal{R}(A) + \mathcal{N}(A) = \mathbb{R}^n \iff \mathrm{index}(A) = 1$$

$$A = S \begin{bmatrix} J & \mathrm{O} \\ \mathrm{O} & 0 \end{bmatrix} S^{-1}, \quad A^\# = S \begin{bmatrix} J^{-1} & \mathrm{O} \\ \mathrm{O} & 0 \end{bmatrix} S^{-1}, \quad \mathcal{R}(A^\#) = \mathcal{R}(A)$$

$$A^\# = A^\dagger \iff \mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A)$$

Convergence of GMRES applied to group (GP) systems

Theorem ([Brown, Walker, SIMAX 97])

If $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$, then GMRES gives a solution of $A\boldsymbol{x} = \boldsymbol{b}$ without breakdown for all $\boldsymbol{b} \in \mathcal{R}(A)$ and for all $\boldsymbol{x}_0 \in \mathbb{R}^n$. The solution is $\boldsymbol{x}_0 + A^{\#}\boldsymbol{r}_0 = \boldsymbol{x}_{\#} + (I - A^{\#}A)\boldsymbol{x}_0$.

$$\boldsymbol{x}_* = A^{\dagger}b \in \mathcal{R}(A^{\mathsf{T}}), \quad \boldsymbol{x}_{\#} = A^{\#}b \in \mathcal{R}(A^{\mathsf{T}}), \quad \boldsymbol{x}_* = P_{\mathcal{R}(A^{\mathsf{T}})}\boldsymbol{x}_{\#} = V_1 V_1^{\mathsf{T}} U_1 U_1^{\mathsf{T}} \boldsymbol{x}_{\#}$$

$$\sigma_{min}(V_1^{\mathsf{T}} U_1)\|\boldsymbol{x}_{\#}\| \leq \|\boldsymbol{x}_*\| \leq \|\boldsymbol{x}_{\#}\|$$

GP case for $\boldsymbol{b} \in \mathcal{R}(A)$

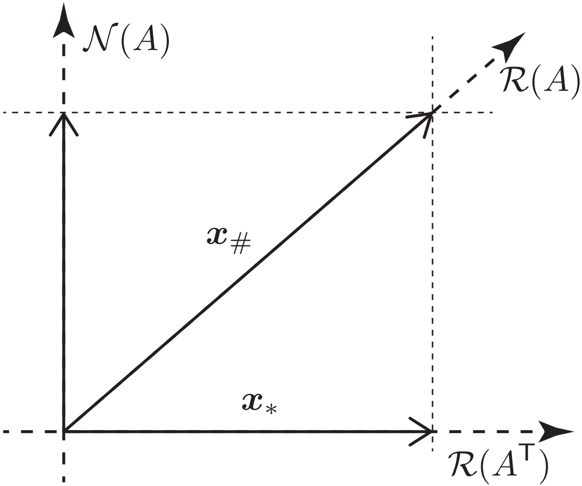


Figure: Geometric illustration of solution vectors.

Group (GP) system, consistent case $\boldsymbol{b} \in \mathcal{R}(A)$

Since $\mathcal{K}_k \subseteq \mathcal{R}(A)$, we have

$$\sigma_k(H_{k+1,k}) = \min_{z \in \mathcal{K}_k \setminus \{\mathbf{0}\}} \frac{\|Az\|}{\|z\|} \geq \min_{z \in \mathcal{R}(A) \setminus \{\mathbf{0}\}} \frac{\|Az\|}{\|z\|}$$

$$\min_{z \in \mathcal{R}(A) \setminus \{\mathbf{0}\}} \frac{\|Az\|}{\|z\|} = \min_{z \in \mathbb{R}^k \setminus \{\mathbf{0}\}} \frac{\|U_1 \Sigma_1 V_1^{\mathsf{T}} U_1 z\|}{\|U_1 z\|} \geq \sigma_{min}(A) \sigma_{min}(V_1^{\mathsf{T}} U_1)$$

Condition number of the Hessenberg matrix $H_{k+1,k}$ depends on the principal angles between $\mathcal{R}(A)$ and $\mathcal{R}(A^{\mathsf{T}})$!

Example: small singular GP system

$$A = \begin{bmatrix} D & \mathrm{I} \\ \mathrm{O} & \mathrm{O} \end{bmatrix} \in \mathbb{R}^{128\times 128}, \quad \boldsymbol{b} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{0} \end{bmatrix}$$

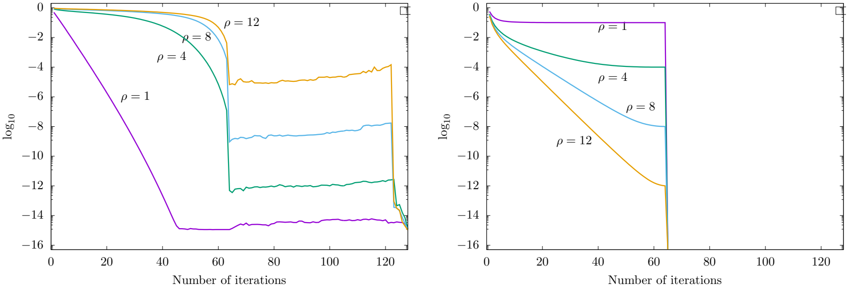
D is a diagonal matrix whose values of the diagonal entries have the so-called Strakoš distribution [Strakoš, LAA 91]

$$d_{1,1} = 1, \quad d_{64,64} = 10^{-\rho}, \quad d_{j,j} = d_{64,64} + \frac{64 - j}{63}(d_{1,1} - d_{64,64}) \cdot 0.7^{j-1},$$

$\boldsymbol{f} = \{f_i\} \in \mathbb{R}^r$ has the entries $f_{r-i+1} = 10^{-(i-1)\rho/63}$. For $\rho \gg 1$,

$$\kappa(A) = \sqrt{2/(10^{-\rho} + 1)} \simeq \sqrt{2},$$
$$\kappa(V_1^{\mathsf{T}} U_1) = 10^{\rho} \sqrt{(10^{-2\rho} + 1)/2} \simeq 10^{\rho}/\sqrt{2}.$$

Example: GMRES



(a) Relative residual norm $\|\boldsymbol{r}_k\|/\|\boldsymbol{b}\|$. (b) Smallest singular value of $H_{k+1,k}$.

Figure: Different condition numbers of $V_1^{\mathsf{T}} U_1$.

Thank you for your attention!

Morikuni Keiichi, R: On GMRES for singular EP and GP systems, SIAM Journal on Matrix Analysis and Applications 39 (2), 2018, 1033-1048.