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Abstract

In this contribution we study the numerical behavior of the Generalized Minimal Residual (GMRES) method for solving singular linear systems. It is known that GMRES determines a solution without breakdown if the coefficient matrix is symmetric in its range (EP); or if its range and nullspace are disjoint (GP). We show that the accuracy of GMRES iterates may in practice deteriorate due to three distinct factors: (i) the inconsistency of a linear system; (ii) the distance of the initial residual to the nullspace of the coefficient matrix; (iii) large principal angles between the ranges of the coefficient matrix and of its transpose. These factors lead to poor conditioning of the extended Hessenberg matrix in the Arnoldi decomposition and affect the accuracy of computed least squares solution. We compare GMRES with the range restricted GMRES (RR-GMRES) method and the simpler GMRES method. Numerical experiments show typical behaviors of GMRES for small problems with EP and GP matrices.

1 Introduction

Consider solving linear systems of equations

$$A\boldsymbol{x} = \boldsymbol{b}, \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$ may be singular and $\boldsymbol{b} \in \mathbb{R}^n$ is not necessarily in $\mathcal{R}(A) = \{\boldsymbol{y} \in \mathbb{R}^n \mid \boldsymbol{y} = A\boldsymbol{x},\ \boldsymbol{x} \in \mathbb{R}^n\}$, the range of A. We say that $A\boldsymbol{x} = \boldsymbol{b}$ is consistent if $\boldsymbol{b} \in \mathcal{R}(A)$, and otherwise it is inconsistent. If (1.1) is inconsistent, instead of (1.1), it is natural to consider solving the least squares problem

$$\|\boldsymbol{b} - A\boldsymbol{x}\| = \min_{\boldsymbol{u}\in\mathbb{R}^n} \|\boldsymbol{b} - A\boldsymbol{u}\|, \tag{1.2}$$

where $\|\cdot\|$ denotes the Euclidean norm. We call a minimizer $\boldsymbol{x} \in \operatorname{argmin}_{\boldsymbol{u}\in\mathbb{R}^n} \|\boldsymbol{b} - A\boldsymbol{u}\|$ a least squares solution, which is not necessarily unique.

We will analyze iterative methods for solving (1.1) in terms of the spaces associated with A and prepare some required definitions and notations. If $\mathcal{N}(A) = \{\boldsymbol{x} \in \mathbb{R}^n \mid A\boldsymbol{x} = \boldsymbol{0}\}$ is the nullspace of A, we have $\mathcal{N}(A^\mathsf{T}) \oplus \mathcal{R}(A) = \mathcal{N}(A) \oplus \mathcal{R}(A^\mathsf{T}) = \mathbb{R}^n$, $\dim \mathcal{N}(A^\mathsf{T}) = \dim \mathcal{N}(A)$, and $\dim \mathcal{R}(A^\mathsf{T}) = \dim \mathcal{R}(A) = \operatorname{rank}(A)$, where $\oplus$ denotes the direct sum of subspaces. Let $r = \operatorname{rank}(A)$ and denote the singular value decomposition (SVD) of A by $U\Sigma V^\mathsf{T}$, where $U \in \mathbb{R}^{n\times n}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices $U^\mathsf{T}U = UU^\mathsf{T} = V^\mathsf{T}V = VV^\mathsf{T} = \mathrm{I}$, I is the identity matrix, $\Sigma = \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r, 0, 0, \ldots, 0) \in \mathbb{R}^{n\times n}$, and σ_i is the ith largest nonzero singular value of A. Let $U = [U_1, U_2]$ and $V = [V_1, V_2]$ be partitioned, where the columns of $U_1 \in \mathbb{R}^{n\times r}$

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and $U_2 \in \mathbb{R}^{n\times(n-r)}$ form orthonormal bases of $\mathcal{R}(A) = \mathcal{R}(U_1)$ and $\mathcal{R}(A)^\perp = \mathcal{N}(A^\mathsf{T}) = \mathcal{R}(U_2)$, respectively, and the columns of $V_1 \in \mathbb{R}^{n\times r}$ and $V_2 \in \mathbb{R}^{n\times(n-r)}$ form orthonormal bases of $\mathcal{N}(A)^\perp = \mathcal{R}(A^\mathsf{T}) = \mathcal{R}(V_1)$ and $\mathcal{N}(A) = \mathcal{R}(V_2)$, respectively. If $\Sigma_r = \mathrm{diag}(\sigma_1, \sigma_2, \cdots \sigma_r)$, we call $A^\dagger = V_1\Sigma_r^{-1}{U_1}^\mathsf{T}$ the Moore-Penrose generalized inverse of A. The condition number of A is denoted by $\kappa(A) = \|A\|\|A^\dagger\|$.

For convenience below, we define the index and the group inverse of a matrix. The smallest nonnegative integer k such that $\mathrm{rank}(A^k) = \mathrm{rank}(A^{k+1})$ is called the index of A [6, Definition 7.2.1], and is denoted by $\mathrm{index}(A)$. In addition, $k \geq \mathrm{index}(A) \iff \mathcal{N}(A^k) + \mathcal{R}(A^k) = \mathbb{R}^n$ [6, p. 137]. Let $\mathrm{index}(A) = 1$ and $X \in \mathbb{R}^{n\times n}$ be such that $AXA = A$, $XAX = X$, and $AX = XA$. Then, X is unique, and we call X the group inverse of A and denote it by $A^\#$. The group inverse can be characterized by the Jordan canonical form. If there exists a nonsingular matrix S such that $J = S^{-1}AS$ is the Jordan canonical form of A, then $A^\# = SJ^\dagger S^{-1}$. In particular, we have $\mathcal{R}(A^\#) = \mathcal{R}(A)$, $\mathcal{N}(A^\#) = \mathcal{N}(A)$, and $A^\#A = AA^\# = P_{\mathcal{R}(A),\mathcal{N}(A)}$ [3].

Now, we express solutions of eqs. (1.1) and (1.2). The solution $\boldsymbol{x}_* = A^\dagger\boldsymbol{b} = V_1\Sigma_r^{-1}U_1^\mathsf{T}\boldsymbol{b}$ of (1.1) or (1.2) is unique and is called the minimum-norm least squares or pseudoinverse solution, which belongs to $\mathcal{R}(A^\mathsf{T})$. We next give the expressions of the residual of (1.2). Denote the orthogonal projector onto $\mathcal{R}(A)$ by $P_{\mathcal{R}(A)} = U_1U_1^\mathsf{T}$ and that onto $\mathcal{N}(A^\mathsf{T})$ by $P_{\mathcal{N}(A^\mathsf{T})} = U_2U_2^\mathsf{T}$. For any $\boldsymbol{x}_0 \in \mathbb{R}^n$ and any $\boldsymbol{b} \in \mathbb{R}^n$, the corresponding residual of (1.2) is $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0 = \boldsymbol{b}|_{\mathcal{N}(A^\mathsf{T})} + \boldsymbol{b}_{\mathcal{R}(A)} - A\boldsymbol{x}_0 = \boldsymbol{r}_* + \boldsymbol{r}_0|_{\mathcal{R}(A)}$, where $\boldsymbol{r}_* = \boldsymbol{b}|_{\mathcal{N}(A^\mathsf{T})} = P_{\mathcal{N}(A^\mathsf{T})}\boldsymbol{b} \in \mathcal{N}(A^\mathsf{T})$ is the least squares residual and $\boldsymbol{b}|_{\mathcal{R}(A)} = P_{\mathcal{R}(A)}\boldsymbol{b}$. In particular, we have $\boldsymbol{r}_* = \boldsymbol{0}$ for $\boldsymbol{b} \in \mathcal{R}(A)$. Assume $\mathrm{index}(A) = 1$. It holds that $\boldsymbol{x}_\# = A^\#\boldsymbol{b}$ is a solution of $A\boldsymbol{x} = \boldsymbol{b} \iff \boldsymbol{b} \in \mathcal{R}(A)$ [6], and it is a unique solution of $A\boldsymbol{x} = \boldsymbol{b}$ in $\mathcal{R}(A)$. Furthermore, the minimum Euclidean norm solution of (1.2) satisfies $\boldsymbol{x}_* = P_{\mathcal{R}(A^\mathsf{T})}\boldsymbol{x}_\#$.

In this paper, we are interested in the numerical behavior of the Generalized Minimal Residual (GMRES) method [16] applied in particular to singular systems (1.1). In section 2, we give some well-known conditions under which GMRES determines a solution without breakdown when applied to certain classes of singular matrices. We discuss also a relation to the range-restricted GMRES (RR-GMRES) method proposed in [5]. In section 3, we examine the conditioning of the coefficient matrix A restricted to the Krylov subspaces that significantly influences the numerical behavior of GMRES. We consider first the case of EP (equal projection) or range-symmetric matrices and distinguish between the consistent and inconsistent cases showing that the consistent case is similar to the nonsingular case. Then we discuss the inconsistent EP case where GMRES suffers from an instability, since the convergence means ill-conditioned restriction of A to the Krylov subspaces. In section 4 we study the case of group projection (GP) matrices. We show that the numerical behavior of GMRES applied to such problems depends substantially on the principal angles between the subspaces $\mathcal{R}(A)$ and $\mathcal{R}(A^\mathsf{T})$. Surprisingly, difficulties can be expected for range-nonsymmetric problems even for consistent systems. In section 5, we conclude the paper.

2 GMRES methods and its convergence for singular systems

GMRES for the linear system (1.1) with initial iterate $\boldsymbol{x}_0 \in \mathbb{R}^n$, independent of any particular implementation of the algorithm, determines the kth iterate $\boldsymbol{x}_k$ over $\boldsymbol{x}_0 + \mathcal{K}_k(A, \boldsymbol{r}_0)$ that minimizes $\|\boldsymbol{b} - A\boldsymbol{x}_k\|$, where $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ is the initial residual and $\mathcal{K}_k(A, \boldsymbol{r}_0) = \mathrm{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{k-1}\boldsymbol{r}_0\}$ is the Krylov subspace of order k. Note that there exist $\boldsymbol{x}_k$ and hence $\boldsymbol{r}_k = \boldsymbol{b} - A\boldsymbol{x}_k$ for all $k \geq 0$ but $\boldsymbol{x}_k$ may not be unique in the singular case. Denote $\mathcal{K}_k(A, \boldsymbol{r}_0)$ by $\mathcal{K}_k$ for simplicity. It is clear that $\mathcal{K}_k = \mathrm{span}\{\boldsymbol{r}_0\} \cup A\mathcal{K}_{k-1} \subset \mathrm{span}\{\boldsymbol{r}_*\} + \mathcal{R}(A)$

holds. If $\dim A\mathcal{K}_k = \dim \mathcal{K}_k$, then the problem

$$\|\boldsymbol{b} - A\boldsymbol{x}_k\| = \min_{\boldsymbol{z}\in\mathcal{K}_k} \|\boldsymbol{b} - A(\boldsymbol{x}_0 + \boldsymbol{z})\| = \min_{\boldsymbol{z}\in\mathcal{K}_k} \|\boldsymbol{r}_0 - A\boldsymbol{z}\| = \|\boldsymbol{r}_0 - A\boldsymbol{z}_k\| \tag{2.1}$$

has a unique solution $\boldsymbol{x}_k = \boldsymbol{x}_0 + \boldsymbol{z}_k$ and hence $\boldsymbol{r}_k = \boldsymbol{b} - A\boldsymbol{x}_k \in \boldsymbol{r}_0 + A\mathcal{K}_k$ is uniquely determined.

General studies on Krylov subspace methods in the singular case were done in [12], [18], [25], [17]. Particular studies on GMRES-type methods in the singular case were done in [5], [19], [15], [20], [9]. See [10] for GMRES on ill-posed linear systems, and [26] for GMRES with preconditioning. See also [11] for GMRES and [1] for GMRES with preconditioning in Hilbert spaces.

In the nonsingular case, GMRES determines the solution of $A\boldsymbol{x} = \boldsymbol{b}$ for all $\boldsymbol{b} \in \mathbb{R}^n$ and for all $\boldsymbol{x}_0 \in \mathbb{R}^n$ within n iterations. In the singular case, GMRES may fail to determine a solution of (1.1), and is said to break down at some step k if $\dim A\mathcal{K}_k < \dim \mathcal{K}_k$ or $\dim \mathcal{K}_k < k$ [4, p. 38]. Note that, in general, $\dim A\mathcal{K}_k \le \dim \mathcal{K}_k \le k$ holds for each k.

We give an explicit expression of the iterate $\boldsymbol{x}_k$ for GMRES using the Arnoldi decomposition $AQ_k = Q_{k+1}H_{k+1,k}$, $k = 1, 2, \ldots$, where the columns of $Q_k = [\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_k]$ form an orthonormal basis of the Krylov subspace $\mathcal{K}_k$, and $H_{k+1,k} = \{h_{i,j}\} \in \mathbb{R}^{(k+1)\times k}$ is an extended Hessenberg matrix. Then the iterate is given by $\boldsymbol{x}_k = \boldsymbol{x}_0 + Q_k\boldsymbol{y}_k$ with $\boldsymbol{y}_k = \arg\min_{\boldsymbol{y}\in\mathbb{R}^k} \|\beta\boldsymbol{e}_1 - H_{k+1,k}\boldsymbol{y}\|$, where $\boldsymbol{e}_1$ is the first column of the identity matrix and $\|\boldsymbol{b} - A\boldsymbol{x}_k\| = \|\boldsymbol{r}_0 - AQ_k\boldsymbol{y}_k\| = \|\beta\boldsymbol{e}_1 - H_{k+1,k}\boldsymbol{y}_k\|$.

It is clear that if $h_{i+1,i} \neq 0$ for $i = 1, 2, \ldots, k-1$, the breakdown does not occur until step $k-1$ of GMRES with $\dim A\mathcal{K}_i = i$, or $\operatorname{rank}(H_{i+1,i}) = i$, $i = 1, 2, \ldots, k-1$. At breakdown of GMRES at step k with $h_{k+1,k} = 0$, one of the following cases holds [13, Appendix A] (cf. [4, Theorem 2.2]):

Case I. $\dim A\mathcal{K}_{k+1} = k < \dim \mathcal{K}_{k+1} = k+1$, whereas $\operatorname{rank}(H_{k,k}) = k-1$.

Case II. $\dim A\mathcal{K}_k = k = \dim \mathcal{K}_{k+1} < k+1$, whereas $\operatorname{rank}(H_{k,k}) = k$ (GMRES determines a solution of $A\boldsymbol{x} = \boldsymbol{b}$ at step k).

A variant of GMRES called the range restricted GMRES (RR-GMRES) method was proposed in [5]. RR-GMRES determines the kth iterate by minimizing the same objective function as GMRES over a different Krylov subspace

$$\|\boldsymbol{b} - A\boldsymbol{x}_k^{\mathrm{R}}\| = \min_{\boldsymbol{z}\in\mathcal{K}_k(A,A\boldsymbol{r}_0)} \|\boldsymbol{b} - A(\boldsymbol{x}_0 + \boldsymbol{z})\| = \min_{\boldsymbol{z}\in\mathcal{K}_k(A,A\boldsymbol{r}_0)} \|\boldsymbol{r}_0 - A\boldsymbol{z}\| = \|\boldsymbol{r}_0 - A\boldsymbol{z}_k^{\mathrm{R}}\|.$$

It was shown in [7, Theorem A2] that if RR-GMRES applied to (1.2) breaks down at step m with $\operatorname{rank}(A) = m-1$ and $\dim A\mathcal{K}_m(A, A\boldsymbol{r}_0) = m-1$, then it determines a solution of (1.2). Here, RR-GMRES is said to break down if $A\mathcal{K}_k(A, A\boldsymbol{r}_0) < \mathcal{K}_k(A, A\boldsymbol{r}_0)$ or $\mathcal{K}_k(A, A\boldsymbol{r}_0) < k$.

We give an explicit expression of the RR-GMRES iterate $\boldsymbol{x}_k$ using the Arnoldi decomposition $AQ_k^{\mathrm{R}} = Q_{k+1}^{\mathrm{R}}H_{k+1,k}^{\mathrm{R}}$, $k = 1, 2, \ldots$, where the columns of $Q_k^{\mathrm{R}} = [\boldsymbol{q}_1^{\mathrm{R}}, \boldsymbol{q}_2^{\mathrm{R}}, \ldots, \boldsymbol{q}_k^{\mathrm{R}}]$ form an orthonormal basis of the Krylov subspace $\mathcal{K}_k(A, A\boldsymbol{r}_0)$ with the initial vector $\boldsymbol{q}_1^{\mathrm{R}} = A\boldsymbol{r}_0/\|A\boldsymbol{r}_0\|$, and $H_{k+1,k}^{\mathrm{R}} = \{h_{i,j}^{\mathrm{R}}\} \in \mathbb{R}^{(k+1)\times k}$ is an extended Hessenberg matrix. Then, the iterate is given by $\boldsymbol{x}_k^{\mathrm{R}} = \boldsymbol{x}_0 + Q_k^{\mathrm{R}}\boldsymbol{y}_k^{\mathrm{R}}$ with $\boldsymbol{y}_k^{\mathrm{R}} = \arg\min_{\boldsymbol{y}\in\mathbb{R}^k} \|(Q_{k+1}^{\mathrm{R}})^{\mathsf{T}}\boldsymbol{r}_0 - H_{k+1,k}^{\mathrm{R}}\boldsymbol{y}\|$, where

$$\begin{aligned}
\|\boldsymbol{b} - A\boldsymbol{x}_k^{\mathrm{R}}\|^2 &= \|\boldsymbol{r}_0 - AQ_k^{\mathrm{R}}\boldsymbol{y}_k^{\mathrm{R}}\|^2 \\
&= \|(Q_{k+1}^{\mathrm{R}})^{\mathsf{T}}\boldsymbol{r}_0 - H_{k+1,k}^{\mathrm{R}}\boldsymbol{y}_k^{\mathrm{R}}\|^2 + \|[\mathrm{I} - Q_{k+1}^{\mathrm{R}}(Q_{k+1}^{\mathrm{R}})^{\mathsf{T}}]\boldsymbol{r}_0\|^2 \\
&= \min_{\boldsymbol{y}\in\mathbb{R}^k} \|(Q_{k+1}^{\mathrm{R}})^{\mathsf{T}}\boldsymbol{r}_0 - H_{k+1,k}^{\mathrm{R}}\boldsymbol{y}\|^2 + \|[\mathrm{I} - Q_{k+1}^{\mathrm{R}}(Q_{k+1}^{\mathrm{R}})^{\mathsf{T}}]\boldsymbol{r}_0\|^2.
\end{aligned}$$

The last term is equal to the kth residual norm for the simpler GMRES method [23], which is not larger than the kth residual norm for RR-GMRES, i.e., $\|\boldsymbol{b} - A\boldsymbol{x}_k\| \leq \|\boldsymbol{b} - A\boldsymbol{x}_k^{\mathrm{R}}\|$. Note also that $\|H_{k,k-1}^{\mathrm{R}}\| = \|AQ_{k-1}^{\mathrm{R}}\| \leq \|A[r_0, Q_{k-1}^{\mathrm{R}}]\| = \|H_{k+1,k}\|$ and

$$\sigma_k(H_{k+1,k}) \leq \min_{\boldsymbol{y} \in \mathbb{R}^{k-1} \setminus \{\boldsymbol{0}\}} \frac{\|AQ_{k-1}^{\mathrm{R}}\boldsymbol{y}\|}{\|Q_{k-1}^{\mathrm{R}}\boldsymbol{y}\|} = \sigma_{k-1}(H_{k,k-1}^{\mathrm{R}})$$

leading to an interesting bound $\kappa(H_{k,k-1}^{\mathrm{R}}) \leq \kappa(H_{k+1,k})$ for $k = 2, \ldots, n-1$.

In the following, we present conditions under which GMRES determines a solution of (1.1). We start with the observation that in the case of $\mathcal{N}(A) \cap \mathcal{R}(A) \neq \{\boldsymbol{0}\}$, GMRES breaks down and fails to determine a solution.

Proposition 2.1. *If $\boldsymbol{b} \in \mathcal{R}(A)$ and $\boldsymbol{r}_0 \in \mathcal{N}(A) \cap \mathcal{R}(A) \neq \{\boldsymbol{0}\}$, then GMRES breaks down at step 1 without determining a solution of $A\boldsymbol{x} = \boldsymbol{b}$.*

Proof. Since $\boldsymbol{r}_0 \neq \boldsymbol{0}$, we have $\dim \mathcal{K}_1 = \dim \operatorname{span}\{\boldsymbol{r}_0\} = 1$. Since $\boldsymbol{r}_0 \in \mathcal{N}(A)$ gives $A\boldsymbol{r}_0 = \boldsymbol{0}$, we have $\dim A\mathcal{K}_1 = \dim \operatorname{span}\{A\boldsymbol{r}_0\} = \dim \operatorname{span}\{\boldsymbol{0}\} = 0$. Hence, $\dim A\mathcal{K}_1 < \dim \mathcal{K}_1$ holds. Therefore, GMRES breaks down at step 1. □

Similarly to GMRES, RR-GMRES also breaks down at step 1 without determining a solution of $A\boldsymbol{x} = \boldsymbol{b}$ if $\boldsymbol{b} \in \mathcal{R}(A)$ and $\boldsymbol{r}_0 \in \mathcal{N}(A) \cap \mathcal{R}(A) \neq \{\boldsymbol{0}\}$. Therefore, we will restrict our attention to the cases of $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\boldsymbol{0}\}$. The following statement holds.

Theorem 2.2 ([4, Theorem 2.6], [25, Theorem 3.2])**.** *If $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\boldsymbol{0}\}$, then GMRES determines 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 $x_{\#} + (\mathrm{I} - A^{\#}A)\boldsymbol{x}_0$.*

The condition $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\boldsymbol{0}\}$ is equivalent to $\operatorname{rank}([U_1, V_2]) = n$, or $\mathcal{R}(U_1) \cap \mathcal{R}(V_2) = \{\boldsymbol{0}\}$ [6, Lemma 7.2.1]. Denote the projection onto $\mathcal{R}(A)$ along $\mathcal{N}(A)$ by $P_{\mathcal{R}(A),\mathcal{N}(A)}$. Then, we have $P_{\mathcal{R}(A),\mathcal{N}(A)} = A^{\#}A = [U_1, \mathrm{O}][U_1, V_2]^{-1} = U_1(V_1^{\mathsf{T}}U_1)^{-1}V_1^{\mathsf{T}}$, because of [3, Exercise 30, p. 148] and

$$[U_1, V_2]^{-1} = \begin{bmatrix} (V_1^{\mathsf{T}}U_1)^{-1} & \mathrm{O} \\ -V_2U_1(V_1^{\mathsf{T}}U_1)^{-1} & \mathrm{I} \end{bmatrix} [V_1, V_2]^{\mathsf{T}}.$$

Thus, $\kappa(A^{\#}A) = \kappa(V_1^{\mathsf{T}}U_1)$ holds.

For a special class of singular matrices, GMRES determines a least squares solution.

Theorem 2.3 ([4, Theorem 2.4])**.** *If $\mathcal{R}(A) = \mathcal{R}(A^{\mathsf{T}})$, then GMRES determines a solution of $\min_{\boldsymbol{x} \in \mathbb{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|$ without breakdown for all $\boldsymbol{b} \in \mathbb{R}^n$ and for all $\boldsymbol{x}_0 \in \mathbb{R}^n$.*

A matrix $A \in \mathbb{R}^{n \times n}$ satisfying $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\boldsymbol{0}\}$, is called a GP (group) matrix. A GP matrix satisfying in addition $\mathcal{R}(A^{\mathsf{T}}) = \mathcal{R}(A)$, or equivalently $\mathcal{R}(U_1) = \mathcal{R}(V_1)$, is called an EP (equal projection) or range-symmetric matrix. Now, we characterize the GP and EP matrices in terms of their singular value decompositions. The matrix A can be decomposed as

$$A = U \begin{bmatrix} \Sigma_r V_1^{\mathsf{T}}U_1 & \Sigma_r V_1^{\mathsf{T}}U_2 \\ \mathrm{O} & \mathrm{O} \end{bmatrix} U^{\mathsf{T}} = V \begin{bmatrix} V_1^{\mathsf{T}}U_1\Sigma_r & \mathrm{O} \\ V_2^{\mathsf{T}}U_1\Sigma_r & \mathrm{O} \end{bmatrix} V^{\mathsf{T}} = V \begin{bmatrix} V_1^{\mathsf{T}}U_1 \\ V_2^{\mathsf{T}}U_1 \end{bmatrix} \Sigma_r V_1^{\mathsf{T}}$$

with the identity $(V_1^{\mathsf{T}}U_1)(V_1^{\mathsf{T}}U_1)^{\mathsf{T}} + (V_1^{\mathsf{T}}U_2)(V_1^{\mathsf{T}}U_2)^{\mathsf{T}} = \mathrm{I}$. The equivalences for GP matrices

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

follow from the equation

$$[V_1, V_2]^\mathsf{T}[U_1, V_2] = \begin{bmatrix} V_1^\mathsf{T}U_1 & \mathrm{O} \\ V_2^\mathsf{T}U_1 & \mathrm{I} \end{bmatrix}.$$

The conditioning of $V_1^\mathsf{T}U_1$ is independent of conditioning of A but it gives a difficulty in solving singular linear systems with GMRES. The EP case $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A)$ is equivalent to that $V_1^\mathsf{T}U_1$ is orthogonal, since $V_1^\mathsf{T}U_2 = \mathrm{O}$.

Next, we characterize GP and EP matrices in terms of the principal angles. In the EP case $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A)$, the matrix $V_1^\mathsf{T}U_1$ is orthogonal and the cosines of the principal angles between $\mathcal{R}(A)$ and $\mathcal{R}(A^\mathsf{T})$ are all zero. In the GP case, since the columns of U_1 and V_1 form bases of $\mathcal{R}(A)$ and $\mathcal{R}(A^\mathsf{T})$, respectively, the cosines of the canonical angles between $\mathcal{R}(A)$ and $\mathcal{R}(A^\mathsf{T})$ are the singular values of $V_1^\mathsf{T}U_1$ [8, section 1.2]. Hence, the condition number of $V_1^\mathsf{T}U_1$ is related to the extremal principal angles.

Note that due to $\|V_1^\mathsf{T}U_1\| \leq 1$ all singular values of $V_1^\mathsf{T}U_1$ are less than or equal to 1 and the number of those equal exactly to 1 gives the dimension of $\mathcal{R}(U_1) \cap \mathcal{R}(V_1)$. So, if $\|V_1^\mathsf{T}U_1\| < 1$, then $\mathcal{R}(U_1) \cap \mathcal{R}(V_1) = \mathcal{R}(A) \cap \mathcal{R}(A^\mathsf{T}) = \{\mathbf{0}\}$. If a matrix $A \in \mathbb{R}^{n\times n}$ satisfies $\mathcal{R}(A) \cap \mathcal{R}(A^\mathsf{T}) = \{\mathbf{0}\}$, it is called a disjoint range (DR) matrix [2].

3 GMRES and EP matrices

As it was already noted, the GMRES iterate $\boldsymbol{x}_k = \boldsymbol{x}_0 + \boldsymbol{z}_k$ solves the least squares problem (2.1). Therefore, the restriction of A to the Krylov subspace $\mathcal{K}_k \subseteq \mathbb{R}^n$ denoted by $A|_{\mathcal{K}_k}$ plays an important role in the numerical behavior of GMRES. Indeed, the ill-conditioning of $A|_{\mathcal{K}_k}$ was studied and its condition number

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

was introduced by Brown and Walker in [4]. In practical computations, the iterate $\boldsymbol{x}_k$ is computed as $\boldsymbol{x}_k = \boldsymbol{x}_0 + Q_k\boldsymbol{y}_k$, where the columns of Q_k form an orthonormal basis of the Krylov subspace $\mathcal{K}_k$ and the vector $\boldsymbol{y}_k$ is a solution of the extended Hessenberg least squares problem $\min_{\boldsymbol{y}\in\mathbb{R}^k} \|\beta\boldsymbol{e}_1 - H_{k+1,k}\boldsymbol{y}\|$ (see section 2). The accuracy of $\boldsymbol{x}_k$ is thus affected directly by the conditioning of the matrix $H_{k+1,k}$, whereas the identity $\kappa(H_{k+1,k}) = \kappa(A|_{\mathcal{K}_k})$ follows from the identities

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

Next, we give bounds on the extremal singular values of $H_{k+1,k}$. The norm of the matrix $H_{k+1,k}$ can be always bounded above by that of A

$$\|H_{k+1,k}\| = \max_{\boldsymbol{z}\in\mathcal{K}_k\setminus\{\mathbf{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \leq \max_{\boldsymbol{z}\in\mathrm{span}\{\boldsymbol{r}_*\}\cup\mathcal{R}(A)\setminus\{\mathbf{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \leq \max_{\boldsymbol{z}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \|A\|.$$

This approach cannot be used to bound the kth (or smallest) singular value of $H_{k+1,k}$ due to

$$\sigma_k(H_{k+1,k}) = \min_{\boldsymbol{z}\in\mathcal{K}_k\setminus\{\mathbf{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \geq \min_{\boldsymbol{z}\in\mathrm{span}\{\boldsymbol{r}_*\}\cup\mathcal{R}(A)\setminus\{\mathbf{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \geq \min_{\boldsymbol{z}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = 0 \tag{3.1}$$

as the last equality holds for A singular.

In the consistent case, the condition number is bounded by $\kappa(H_{k+1,k}) \leq \kappa(A|_{\mathcal{R}(A)})$ from $\mathcal{K}_k \subseteq \mathcal{R}(A)$ and

$$\sigma_k(H_{k+1,k}) \geq \min_{\boldsymbol{z} \in \mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|},$$

where $A|_{\mathcal{R}(A)}$ denotes the restriction of A to the range $\mathcal{R}(A)$. If A is an EP matrix $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A)$, then

$$\min_{\boldsymbol{z} \in \mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \min_{\boldsymbol{z} \in \mathcal{R}(A^\mathsf{T})\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \sigma_r(A) > 0$$

and

$$\kappa(A|_{\mathcal{R}(A)}) = \frac{\|A\|}{\min_{\boldsymbol{z} \in \mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \|A\boldsymbol{z}\|/\|\boldsymbol{z}\|} = \kappa(A).$$

Indeed, the consistent EP case is similar to the nonsingular case, and the condition number of the extended Hessenberg matrix $H_{k+1,k}$ is bounded by $\kappa(H_{k+1,k}) \leq \kappa(A)$ (cf. [27, Remark 3.2, Theorem 3.6]). Consequently, the rank deficiency of the least squares problem (2.1) cannot occur and GMRES will terminate if a solution is reached at some step with a degeneracy of the Krylov subspace at the next step.

In the inconsistent EP case, the equivalence $\mathcal{R}(A^\mathsf{T}) = \mathcal{R}(A) \iff \mathcal{N}(A^\mathsf{T}) = \mathcal{N}(A)$ shows that the nonzero least squares residual $\boldsymbol{r}_* \in \mathcal{N}(A^\mathsf{T})$ belongs also to $\mathcal{N}(A)$ and

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

It follows from (2.1) that the residual $\boldsymbol{r}_{k-1}$ at step $k-1$ belongs to the Krylov subspace $\mathcal{K}_k$ and satisfies $\boldsymbol{r}_{k-1} - \boldsymbol{r}_* \in \mathcal{R}(A)$. In addition, due to $A\boldsymbol{r}_* = \boldsymbol{0}$ we have

$$\begin{aligned} \sigma_k(H_{k+1,k}) &= \min_{\boldsymbol{z} \in \mathcal{K}_k\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \leq \frac{\|A\boldsymbol{r}_{k-1}\|}{\|\boldsymbol{r}_{k-1}\|} \\ &= \frac{\|A(\boldsymbol{r}_{k-1} - \boldsymbol{r}_*)\|}{\|\boldsymbol{r}_{k-1}\|} \leq \|A\| \frac{\|\boldsymbol{r}_{k-1} - \boldsymbol{r}_*\|}{\|\boldsymbol{r}_{k-1}\|}. \end{aligned} \tag{3.2}$$

This result was derived in a somewhat different form in [4, Theorem 2.5]. It is clear that in the inconsistent case, the least squares problem (2.1) becomes ill-conditioned as the GMRES iterate converges to a least squares solution. This situation is illustrated in Figure 3.1. Note also that (3.2) can be written for the step $k = 1$ as

$$\sigma_k(H_{k+1,k}) \leq \frac{\|A\boldsymbol{r}_0\|}{\|\boldsymbol{r}_0\|} \leq \frac{\|A\|\|\boldsymbol{r}_0|_{\mathcal{R}(A^\mathsf{T})}\|}{\|\boldsymbol{r}_0\|} = \frac{\|A\|\|\boldsymbol{r}_0|_{\mathcal{R}(A)}\|}{\|\boldsymbol{r}_0\|}.$$

This bound indicates that if the norm of $A\boldsymbol{r}_0$ is too small, the inaccuracy can be expected at all subsequent steps of GMRES. Note that if $\boldsymbol{r}_0 \in \mathcal{N}(A)$, then GMRES breaks down at step 1 with $\boldsymbol{x}_0$ being the least squares solution of (1.2) (see also Proposition 2.1). Finally, since a symmetric matrix is an EP matrix, the above discussion also covers the MINRES method [14] applied to symmetric singular systems.

The conditioning of the extended Hessenberg matrix $H_{k+1,k}$ for GMRES and its relation to conditioning of A are illustrated on small examples. First for simplicity, consider applying GMRES with $\boldsymbol{x}_0 = \boldsymbol{0}$ to $A\boldsymbol{x} = \boldsymbol{b}$, where

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ \varepsilon \end{bmatrix} \tag{3.3}$$

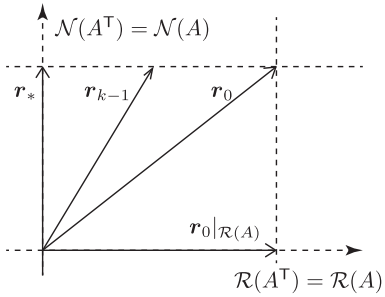


Figure 3.1: Geometric illustration of residual vectors in the EP case.

for $\varepsilon > 0$. The matrix A is EP, it has the range $\mathcal{R}(A) = \mathcal{R}(A^\mathsf{T}) = \mathrm{span}\{[1,0]^\mathsf{T}\}$ and the nullspace $\mathcal{N}(A) = \mathcal{N}(A^\mathsf{T}) = \mathrm{span}\{[0,1]^\mathsf{T}\}$, and its minimum nonzero singular value is $\sigma_1(A) = \min_{\boldsymbol{z}\in\mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \|A\boldsymbol{z}\|/\|\boldsymbol{z}\| = 1$. The first two steps of the Arnoldi process for A and the initial vector $\boldsymbol{q}_1 = \boldsymbol{b}/\|\boldsymbol{b}\|$ give the decomposition $AQ_2 = Q_2H_{2,2}$, where

$$Q_2 = [\boldsymbol{q}_1, \boldsymbol{q}_2] = \frac{1}{\sqrt{1+\varepsilon^2}}\begin{bmatrix} 1 & \varepsilon \\ \varepsilon & -1 \end{bmatrix}, \quad H_{2,2} = \frac{1}{1+\varepsilon^2}\begin{bmatrix} 1 & \varepsilon \\ \varepsilon & \varepsilon^2 \end{bmatrix}.$$

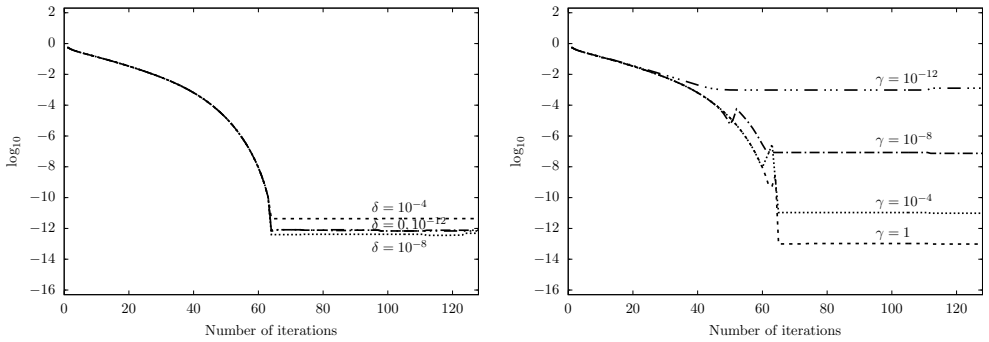
Hence, $H_{2,2}$ is singular and we have $\sigma_1(A) = \sigma_1(H_{2,1}) = \sigma_1(H_{2,2}) = 1$. Solving $\min_{\boldsymbol{y}\in\mathbb{R}^2} \|\beta\boldsymbol{e}_1 - H_{2,2}\boldsymbol{y}\| = \varepsilon$, where $\beta = \sqrt{1+\varepsilon^2}$, we have $\boldsymbol{y}_2 = [\sqrt{1+\varepsilon^2}, 0]^\mathsf{T}$ and $\|\boldsymbol{y}_2\| = \sqrt{1+\varepsilon^2}$. Therefore, $\boldsymbol{x}_2 = [1,\varepsilon]^\mathsf{T}$ and thus the norm of the iterate does not represent a problem here. It is also clear that for $\varepsilon = 0$ the system (3.3) becomes consistent and then GMRES will deliver the minimum norm solution $\boldsymbol{x}_* = [1,0]^\mathsf{T}$ in one iteration.

In the following numerical examples, we examine the accuracy of the GMRES iterate due to the consistency of linear systems by using the test matrix and right hand side vectors

$$A = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{128\times 128}, \quad \boldsymbol{b} = \begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\delta} \end{bmatrix}, \tag{3.4}$$

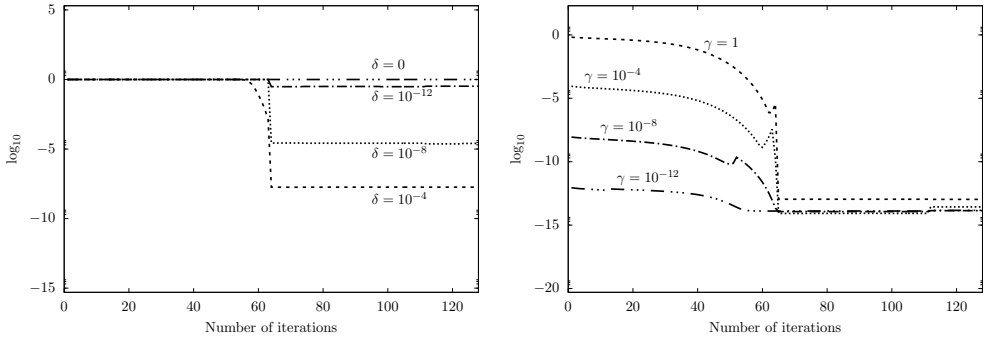
where $D = \mathrm{diag}(10^{\frac{0}{127}}, 10^{\frac{-4}{127}}, 10^{\frac{-8}{127}}, \ldots, 10^{-4}) \in \mathbb{R}^{64\times 64}$, $\boldsymbol{\gamma} = [\gamma, \gamma, \ldots, \gamma]^\mathsf{T} \in \mathbb{R}^{64}$ and $\boldsymbol{\delta} = [\delta, \delta, \ldots, \delta]^\mathsf{T} \in \mathbb{R}^{64}$. Hence, A has the condition number 10^4, and $\boldsymbol{b} \notin \mathcal{R}(A) \iff \delta \neq 0$. An inconsistency of the linear system $A\boldsymbol{x} = \boldsymbol{b}$ can be controlled by the ratio between γ and δ. Since $\mathcal{R}(A) = \mathcal{R}(A^\mathsf{T})$, GMRES should determine the least squares solution of $\min_{\boldsymbol{x}\in\mathbb{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|$ for all $\boldsymbol{b} \in \mathbb{R}^{128}$ (Theorem 2.3). Throughout all our numerical experiments, we use GMRES and RR-GMRES with the Householder orthogonalization process [22] to ensure the best possible orthogonality among the Arnoldi basis vectors $\boldsymbol{q}_1$, $\boldsymbol{q}_2$, $\ldots$, $\boldsymbol{q}_k$ and we compute the kth residual $\boldsymbol{r}_k = \boldsymbol{b} - A\boldsymbol{x}_k$ explicitly from $\boldsymbol{x}_k$ by solving the extended Hessenberg least squares problem $\min_{\boldsymbol{y}\in\mathbb{R}^k} \|\beta\boldsymbol{e}_1 - H_{k+1,k}\boldsymbol{y}\|$ with the Matlab backslash solver, which utilizes the column pivoting.

Figure 3.2 shows the relative residual norm $\|A^\mathsf{T}\boldsymbol{r}_k\|/\|A^\mathsf{T}\boldsymbol{b}\|$ versus the number of iterations of GMRES in the weakly inconsistent cases $(\gamma,\delta) = (1,0)$, $(1,10^{-12})$, $(1,10^{-8})$, and $(1,10^{-4})$ on the left, and and in the strongly inconsistent cases $(\gamma,\delta) = (1,1)$, $(10^{-4},1)$, $(10^{-8},1)$, and $(10^{-12},1)$ on the right. Similarly, Figures 3.3 and 3.4 show the relative residual error norm $\|\boldsymbol{r}_k - \boldsymbol{r}_*\|/\|\boldsymbol{r}_k\|$ and the extremal singular values of A and $H_{k+1,k}$, respectively. If the inconsistency is small ($\delta \ll \gamma$), then GMRES is sufficiently accurate (Figure 3.2a); otherwise the relative residual norm $\|A^\mathsf{T}\boldsymbol{r}_k\|/\|A^\mathsf{T}\boldsymbol{b}\|$ stagnates before attaining the accuracy on the level of $u\kappa(A)$ (Figure 3.2b). In contrast to nonsingular case, GMRES deteriorates not only due to the condition number of A but also due to the inconsistency measured here by $\delta > 0$. For strongly inconsistent systems



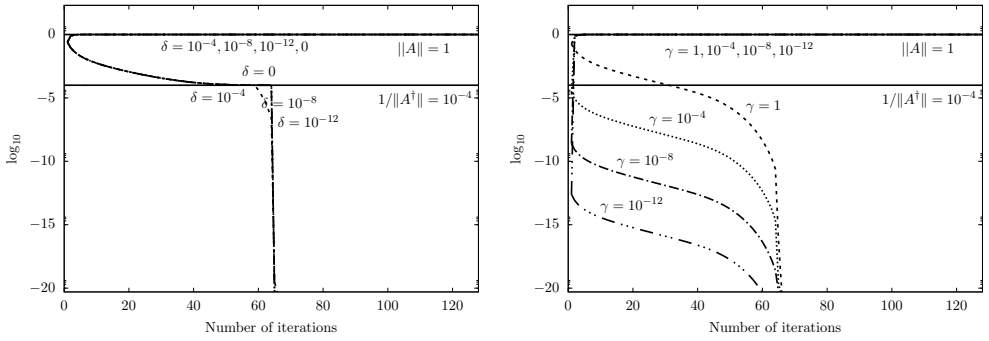
(a) Weakly inconsistent cases ($\gamma = 1$). (b) Strongly inconsistent cases ($\delta = 1$).

Figure 3.2: Relative residual norm $\|A^\mathsf{T}\boldsymbol{r}_k\|/\|A^\mathsf{T}\boldsymbol{b}\|$ for GMRES.



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

Figure 3.3: Relative residual error norm $\|\boldsymbol{r}_k - \boldsymbol{r}_*\|/\|\boldsymbol{r}_k\|$ for GMRES.



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

Figure 3.4: Extremal singular values of A and $H_{k+1,k}$ for GMRES.

with $\delta \gg \gamma$, i.e., for $\boldsymbol{r}_0$ close to $\mathcal{N}(A)$, even though $\|A^\mathsf{T}\boldsymbol{r}_k\|/\|A^\mathsf{T}\boldsymbol{b}\|$ is large and stagnates, and $\|\boldsymbol{r}_*\|$ and hence $\|\boldsymbol{r}_k\|$ are large, the residual $\boldsymbol{r}_k$ approaches $\boldsymbol{r}_*$. Figure 3.4b shows that for strongly inconsistent problems, $H_{k+1,k}$ has a condition number significantly larger than A, tends to be ill-conditioned in the subsequent steps, and is numerically rank-deficient with $u\|H_{k+1,k}\|\|H_{k+1,k}^\dagger\| \geq 1$ within several iterations. In particular, for $\gamma = 0$ and $\delta = 1$, GMRES breaks down at step 1 but gives a least squares solution. Comparing Figures 3.3b and 3.4b, we

see that in these cases the bound (3.2) gives a reasonably good upper estimate for the smallest singular value of $H_{k+1,k}$.

A remedy for the ill-conditioning occurring in GMRES due to inconsistency is to form a Krylov subspace by starting with the initial vector $A\boldsymbol{r}_0$ in $\mathcal{R}(A)$ instead of $\boldsymbol{r}_0$ for the Krylov subspace $\mathcal{K}_k(A, A\boldsymbol{r}_0)$ such as it is done in RR-GMRES. Note that on the other hand, the RR-GMRES residual norm is always larger than or equal to the GMRES residual norm (see section 2). Similarly to the above, we show numerical results for RR-GMRES on the same inconsistent linear systems (3.4). Figures 3.5 to 3.7 show the same quantities as Figures 3.2 to 3.4 for RR-GMRES. For any inconsistency parameter $\delta > 0$, the condition number of $H^R_{k+1,k}$ is bounded above by the condition number of A and RR-GMRES is sufficiently accurate, as

$$\begin{aligned}\sigma_k(H^{\mathrm{R}}_{k+1,k}) &= \min_{\boldsymbol{z}\in\mathcal{K}_k(A,A\boldsymbol{r}_0)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \\ &\geq \min_{\boldsymbol{z}\in\mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \min_{\boldsymbol{z}\in\mathcal{R}(A^{\mathsf{T}})\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \sigma_r(A)\end{aligned}$$

for $\mathcal{R}(A) = \mathcal{R}(A^{\mathsf{T}})$. Thus, the accuracy of the RR-GMRES iterate is affected only by the condition number of A, even though the inconsistency increases or $\boldsymbol{r}_0$ approaches $\mathcal{N}(A)$. Hence, for inconsistent problems with EP matrices RR-GMRES is a successful alternative to GMRES.

4 GMRES and GP matrices

We have shown in section 3 that the condition number $\kappa(A|_{\mathcal{R}(A)})$ plays an important role in the behavior of GMRES and in the EP case we have $\kappa(A|_{\mathcal{R}(A)}) = \kappa(A)$. Thus for consistent problems with EP matrices, the condition number of A represents an upper bound for the condition number of $H_{k+1,k}$ due to $\kappa(H_{k+1,k}) \leq \kappa(A|_{\mathcal{R}(A)}) = \kappa(A)$ and the accuracy of the GMRES iterates is actually determined by the spectral properties of A. Consider now applying GMRES to $A\boldsymbol{x} = \boldsymbol{b}$, where A is a GP matrix (Theorem 2.2). We will show that in the GP case $\kappa(A|_{\mathcal{R}(A)})$ can be significantly larger than $\kappa(A)$ and thus the condition number $\kappa(H_{k+1,k})$ can become larger than $\kappa(A)$ even in the consistent case. The accuracy of the GMRES iterates can be then affected by the inaccurate solution of the extended Hessenberg least squares problem that can be ill-conditioned even if A is well-conditioned.

According to Theorem 2.2, GMRES in the consistent GP case determines $\boldsymbol{x}_{\#} + (\mathrm{I} - A^{\#}A)\boldsymbol{x}_0$. The vector $\boldsymbol{x}_{\#}$ that belongs to $\mathcal{R}(A)$ can be related to the vector $\boldsymbol{x}_*$ that belongs to $\mathcal{R}(A^{\mathsf{T}})$ as follows:

$$\sigma_r(V_1^{\mathsf{T}}U_1)\|\boldsymbol{x}_{\#}\| \leq \|\boldsymbol{x}_*\| \leq \|\boldsymbol{x}_{\#}\|, \tag{4.1}$$

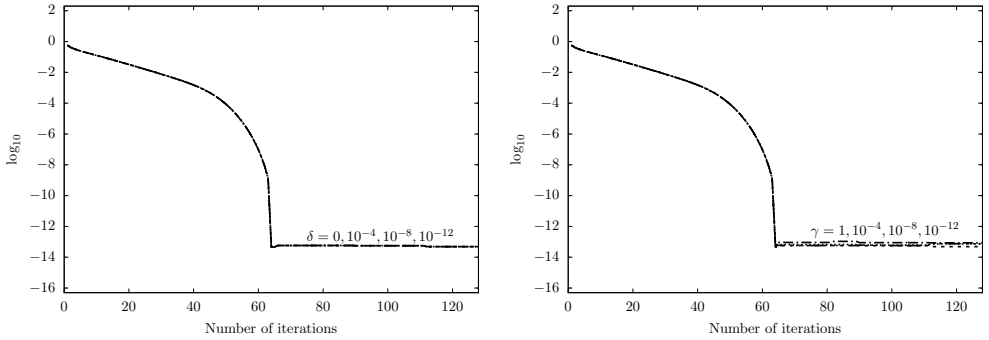
which follows from the identity $\boldsymbol{x}_* = P_{\mathcal{R}(A^{\mathsf{T}})}\boldsymbol{x}_{\#} = V_1V_1^TU_1U_1^Tx_{\#}$. Note that $\boldsymbol{x}_{\#}$ has a large component in $\mathcal{N}(A)$ which may affect the accuracy of GMRES iterates (see Figure 4.1).

In the consistent case, the extremal singular values of $H_{k+1,k}$ can be bounded as

$$\sigma_1(H_{k+1,k}) \leq \max_{\boldsymbol{z}\in\mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \max_{\boldsymbol{z}\in\mathbb{R}^k\setminus\{\boldsymbol{0}\}} \frac{\|U_1\Sigma_1V_1^{\mathsf{T}}U_1\boldsymbol{z}\|}{\|U_1\boldsymbol{z}\|} \leq \|A\|\|V_1^{\mathsf{T}}U_1\|,$$

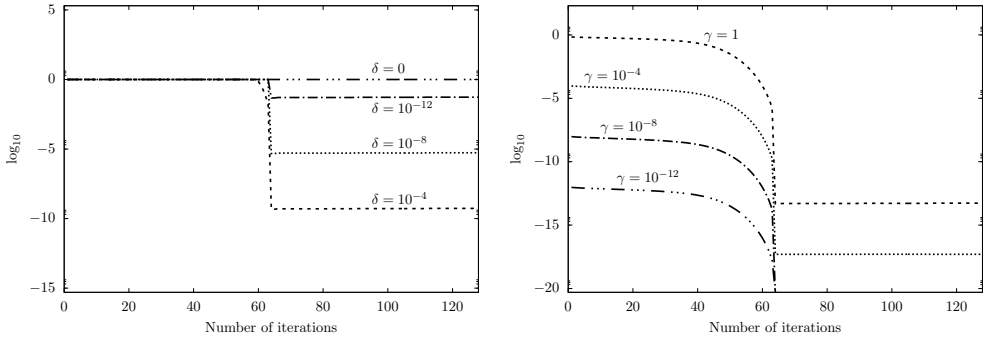
$$\sigma_k(H_{k+1,k}) \geq \min_{\boldsymbol{z}\in\mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \min_{\boldsymbol{z}\in\mathbb{R}^k\setminus\{\boldsymbol{0}\}} \frac{\|U_1\Sigma_1V_1^{\mathsf{T}}U_1\boldsymbol{z}\|}{\|U_1\boldsymbol{z}\|} \geq \sigma_r(A)\sigma_r(V_1^{\mathsf{T}}U_1). \tag{4.2}$$

Consequently, $\kappa(H_{k+1,k}) \leq \kappa(A)\kappa(V_1^{\mathsf{T}}U_1)$ is related to the extremal principal angles between $\mathcal{R}(A)$ and $\mathcal{R}(A^{\mathsf{T}})$ (cf. [24, Theorem 2.1]). The lower bound (4.2) shows that in the consistent



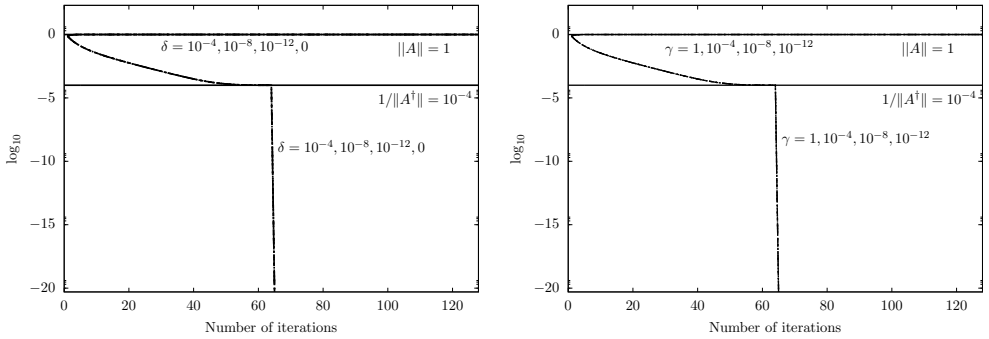
(a) Weakly inconsistent cases ($\gamma = 1$). (b) Strongly inconsistent cases ($\delta = 1$).

Figure 3.5: Relative residual norm $\|A^{\mathsf{T}}\boldsymbol{r}_k^{\mathrm{R}}\|/\|A^{\mathsf{T}}\boldsymbol{b}\|$ for RR-GMRES.



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

Figure 3.6: Relative residual error norm $\|\boldsymbol{r}_k^{\mathrm{R}} - \boldsymbol{r}_*\|/\|\boldsymbol{r}_k^{\mathrm{R}}\|$ for RR-GMRES.



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

Figure 3.7: Extremal singular values of A and $H_{k+1,k}^{\mathrm{R}}$ for RR-GMRES.

case the smallest singular value of $H_{k+1,k}$ can be smaller than the nonzero one of A, depending on that of $V_1^{\mathsf{T}}U_1$. In addition, it is easy to see that $\sigma_k(H_{k+1,k})$ can be bounded by

$$\sigma_k(H_{k+1,k}) = \min_{\boldsymbol{z}\in\mathcal{K}_k\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} \leq \frac{\|A\boldsymbol{r}_0\|}{\|\boldsymbol{r}_0\|} \leq \frac{\|A\|\|\boldsymbol{r}_0|_{\mathcal{R}(A^{\mathsf{T}})}\|}{\|\boldsymbol{r}_0\|}.$$

Here, the last inequality is implied by the splitting $A\boldsymbol{r}_0 = A(\boldsymbol{r}_0|_{\mathcal{N}(A)} + \boldsymbol{r}_0|_{\mathcal{R}(A^{\mathsf{T}})}) = A\boldsymbol{r}_0|_{\mathcal{R}(A^{\mathsf{T}})}$.

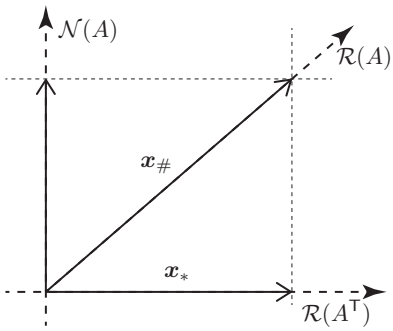


Figure 4.1: Geometric illustration fo solution vectors in the GP case.

Although Brown and Walker mention in [4, p. 50] that the condition number of $A|_{\mathcal{K}_k}$ cannot become arbitrarily large through an unfortunate choice of $\boldsymbol{b}$ and $\boldsymbol{x}_0$, it is clear that if the residual $\boldsymbol{r}_0$ has a very small component in $\mathcal{R}(A^\mathsf{T})$ then such situation can be achieved for any singular matrix A.

In the following, we give illustrative examples that lead to ill-conditioned extended Hessenberg matrix $H_{k+1,k}$ in GMRES. First, we consider GMRES with $\boldsymbol{x}_0 = \boldsymbol{0}$ applied to $A\boldsymbol{x} = \boldsymbol{b}$, where

$$A = \begin{bmatrix} \varepsilon & 1 \\ 0 & 0 \end{bmatrix}, \quad A^\# = \begin{bmatrix} 1/\varepsilon & 1/\varepsilon^2 \\ 0 & 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

The matrix A has the following range and nullspace

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

It is clear that for $\varepsilon = 0$ the matrix A is DR. In addition, the initial vector $\boldsymbol{r}_0$ satisfies $\boldsymbol{r}_0 \in \mathcal{N}(A) \cap \mathcal{R}(A)$ and thus the GMRES method breaks down at step 1. Now suppose that $0 < \varepsilon \ll 1$. Then, the matrix A is GP but not EP ($\mathcal{R}(A^\mathsf{T}) \neq \mathcal{R}(A)$), and because $\sigma_1(V_1^\mathsf{T} U_1) = \varepsilon$ we have

$$\min_{\boldsymbol{z} \in \mathcal{R}(A)\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \varepsilon, \qquad \min_{\boldsymbol{z} \in \mathcal{R}(A^\mathsf{T})\setminus\{\boldsymbol{0}\}} \frac{\|A\boldsymbol{z}\|}{\|\boldsymbol{z}\|} = \sqrt{1+\varepsilon^2}.$$

The smallest singular value of $H_{2,1}$ is significantly smaller than the smallest nonzero singular value of A, $\sigma_1(H_{2,1}) = \varepsilon \ll \sqrt{1+\varepsilon^2} = \sigma_1(A)$. Indeed, the components of $H_{2,1}$ are $H_{2,1} = [\varepsilon, 0]^\mathsf{T}$. Furthermore, by solving $\min_{\boldsymbol{y} \in \mathbb{R}^1} \|\beta \boldsymbol{e}_1 - H_{2,1}\boldsymbol{y}\|$ with $\beta = 1$, we have $\boldsymbol{y}_1 = 1/\varepsilon$, i.e., $\boldsymbol{y}_1$ has a large component. We see that $\boldsymbol{x}_1 = Q_1 \boldsymbol{y}_1$ and $\boldsymbol{x}_1 = \boldsymbol{x}_\# = A^\# \boldsymbol{b} = [1/\varepsilon, 0]^\mathsf{T}$ for $\boldsymbol{b} = [1, 0]^\mathsf{T}$. Therefore, $\|\boldsymbol{x}_1\|$ becomes very large even if the condition number of A and the norm of the right-hand side are small. Indeed, the vector $\boldsymbol{x}_* = 1/(1+\varepsilon^2)[\varepsilon, 1]^T$ and thus the vector $x_\#$ contains a large component in $\mathcal{N}(A)$ and satisfies the inequalities (4.1).

Note that if we consider the inconsistent system with the right hand side $\boldsymbol{b} = [\varepsilon, 1]^T$, then GMRES method will break down in the second step with

$$Q_2 = [\boldsymbol{q}_1, \boldsymbol{q}_2] = \frac{1}{\sqrt{1+\varepsilon^2}} \begin{bmatrix} \varepsilon & 1 \\ 1 & -\varepsilon \end{bmatrix}, \quad H_{3,2} = \begin{bmatrix} \varepsilon & 0 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}, \tag{4.3}$$

whereas $\mathrm{rank}(H_{3,2}) = 1 < \mathrm{rank}(Q_2) = 2$ and $\boldsymbol{q}_2 \in N(A)$ (see Case I in section 2).

The above observation is tested on numerical examples $A\boldsymbol{x} = \boldsymbol{b}$ with an even size of A satisfying $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\mathbf{0}\}$ and having the structure:

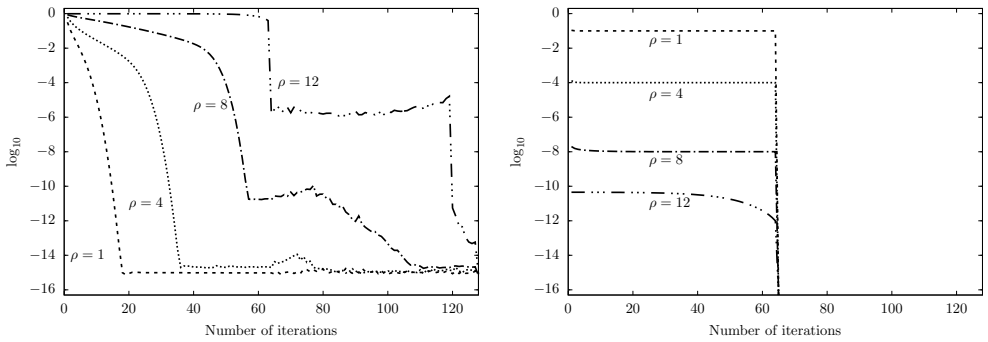
$$A = \begin{bmatrix} D & \mathrm{I} \\ \mathrm{O} & \mathrm{O} \end{bmatrix} \in \mathbb{R}^{128\times 128}, \quad \boldsymbol{b} = \begin{bmatrix} \boldsymbol{f} \\ \mathbf{0} \end{bmatrix}, \tag{4.4}$$

where $D = \{d_{i,j}\}\mathbb{R}^{64\times 64}$ is a diagonal matrix whose values of the diagonal entries have the so-called Strakoš distribution [21]

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

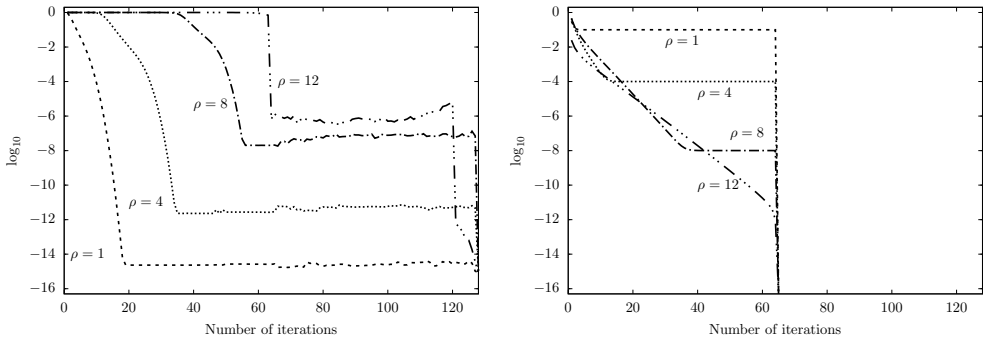
$j = 2, 3, \ldots, 63$, and $\boldsymbol{f} = \{f_i\} \in \mathbb{R}^r$ has the entries $f_{r-i+1} = 10^{-(i-1)\rho/63}$, $i = 1, 2, \ldots, 64$. This setting gives A well-conditioned for $\kappa(A) = \sqrt{2/(10^{-\rho}+1)} \simeq \sqrt{2}$ and $V_1^{\mathsf{T}}U_1$ ill-conditioned for $\kappa(V_1^{\mathsf{T}}U_1) = 10^{\rho}\sqrt{(10^{-2\rho}+1)/2} \simeq 10^{\rho}/\sqrt{2}$ for $\rho \gg 1$. Furthermore, the norms of vectors $\boldsymbol{f}$, $D\boldsymbol{f}$, $D^2\boldsymbol{f}$ decrease and this reduction is pronounced as the value of ρ increases.

Figures 4.2 and 4.3 show the relative residual norm and the smallest singular value of $H_{k+1,k}$ and $H^{\mathrm{R}}_{k+1,k}$ versus the number of iterations for GMRES and RR-GMRES, respectively, applied to the above linear systems with $\rho = 1$, 4, 8, and 12. As the value of ρ increases, the condition number of the extended Hessenberg matrix increases and however the accuracy of the relative residual for both GMRES and RR-GMRES is significantly lost. It is clear from our experiments



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

Figure 4.2: GMRES on (4.4) with $\boldsymbol{b} = [\boldsymbol{f}^{\mathsf{T}}, \mathbf{0}^{\mathsf{T}}]^{\mathsf{T}}$ and different $\kappa(V_1^{\mathsf{T}}U_1) \simeq 10^{\rho}/\sqrt{2}$.



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

Figure 4.3: RR-GMRES on (4.4) with $\boldsymbol{b} = [\boldsymbol{f}^{\mathsf{T}}, \mathbf{0}^{\mathsf{T}}]^{\mathsf{T}}$ and different $\kappa(V_1^{\mathsf{T}}U_1) \simeq 10^{\rho}/\sqrt{2}$.

that while RR-GMRES does help in the inconsistent EP case by starting with a vector in $\mathcal{R}(A)$ to construct the Krylov subspace, in the GP case both GMRES and RR-GMRES may not be accurate for large condition number of $V_1^{\mathsf{T}}U_1$ even in the consistent case.

5 Conclusions

In this paper we have considered the behavior of the GMRES method for solving a linear system $A\boldsymbol{x} = \boldsymbol{b}$, where A is singular. We have discussed two classes of singular matrices (EP and GP) satisfying the conditions under which GMRES converges to a least squares solution and to the group inverse solution, respectively. We have distinguished between the consistent and inconsistent cases and studied the conditioning of the extended Hessenberg least squares problem that can significantly affect the accuracy of approximate solutions computed by GMRES in finite precision arithmetic.

It appears that the consistent EP case is similar to the nonsingular case. The rank deficiency of the extended Hessenberg least squares problem does not occur and GMRES converges to the accurate approximate solution and terminates with a degeneracy of the Krylov space in the next step. If the coefficient matrix is EP, but system $A\boldsymbol{x} = \boldsymbol{b}$ is inconsistent, then despite of the theoretical guarantee to the least squares solution, the extended Hessenberg least squares problem becomes seriously ill-conditioned and this may lead to very inaccurate approximate solutions in GMRES. This happens when the distance of the initial residual to the nullspace is too small or when the residual vector converges gradually to the least squares residual. A remedy is to use RR-GMRES for such cases.

It is known that if the coefficient matrix is GP, then theoretically GMRES converges to the solution given by the group inverse of A. We have shown, however, that the extended Hessenberg least squares problem can be ill-conditioned even in the consistent case. Indeed, the conditioning of the extended Hessenberg matrix $H_{k+1,k}$ in GMRES depends not only on the conditioning of the coefficient matrix A (as it is in the case of consistent EP problems) but also on the smallest principal angle between the spaces $\mathcal{R}(A^{\mathsf{T}})$ and $\mathcal{R}(A)$ that can be quite large. In such cases, both GMRES and RR-GMRES may compute inaccurate approximate solutions.

We believe that under conditions guaranteeing the convergence of GMRES to the generalized least squares solution considered in [25], these results can be extended to singular systems with a general index index(A). Note also that in this paper we assume only exact arithmetic and our considerations form a groundwork for the future rounding error analysis.

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