A stabilized GMRES method for obtaining the minimum-norm solution of inconsistent least squares problems

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Abstract

Consider using the right-preconditioned GMRES for obtaining the minimum-norm solution of underdetermined inconsistent least squares problems. Morikuni (Ph.D. thesis, 2013) showed that for some inconsistent and ill-conditioned problems, the iterates may diverge. This is mainly because the Hessenberg matrix in the GMRES method becomes very ill-conditioned so that the backward substitution of the resulting triangular system becomes numerically unstable. We propose a stabilized GMRES based on solving the normal equations corresponding to the above triangular system using the standard Cholesky decomposition. This has the effect of shifting upwards the tiny singular values of the Hessenberg matrix which lead to an inaccurate solution. Thus, the process becomes numerically stable and the system becomes consistent, rendering better convergence and a more accurate solution. Numerical experiments show that the proposed method is robust and efficient. The method can be considered as a way of making GMRES stable for highly ill-conditioned inconsistent problems.

1 Introduction

Consider obtaining the minimum-norm solution of the inconsistent least squares problem:

\[
\min_{x \in \mathbb{R}^n} \|x\|_2, \text{such that } x \in \{ \arg \min_{\xi \in \mathbb{R}^n} \| b - A\xi \|_2 \}
\]

(1)

where \( A \in \mathbb{R}^{m \times n} \) and \( b \notin \mathcal{R}(A) \subset \mathbb{R}^m \). Here, \( \mathcal{R}(A) \) denotes the range space of \( A \). Such problems may occur in ill-posed problems where \( b \) is given by an observation which contains noise. The problem (1) is equivalent to

\[
(A^T A)^2 u = A^T b, \quad x = A^T A u,
\]

(2)

and the solution can be expressed by \( x = A^\dagger b \), where \( A^\dagger \) is the pseudoinverse of \( A \). (See e.g. [2].)

The standard direct method for solving the least squares problem (1) is to use the QR decomposition. However, when \( A \) is large and sparse, iterative methods become necessary. The CGLS [11] and LSQR [20] are mathematically equivalent to applying the conjugate gradient (CG) method to the normal equations

\[
A^T A x = A^T b,
\]

(3)

which is equivalent to

\[
\min_{x \in \mathbb{R}^n} \| b - A x \|_2.
\]

(4)

CGLS will converge to the minimum-norm solution \( x = A^\dagger b \), provided \( x_0 \in \mathcal{R}(A) \) (See e.g. [2], p.291). However, the convergence of these methods deteriorates for ill-conditioned problems and they require reorthogonalization [10] to improve the convergence. Here, we say (1) is ill-conditioned if the condition number \( \kappa_2(A) = \| A \|_2 \| A^{-1} \|_2 \gg 1 \). The LSMR [17] applies MINRES [19] to (3).

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For the case when $A$ is a square matrix ($m=n$), we mention, for instance [14, 4] for methods for solving nearly singular systems.

Hayami et al. [10] proposed preconditioning the $m \times n$ rectangular matrix $A$ of the least squares problem by an $n \times m$ rectangular matrix $B$ from the right and the left, and using the generalized minimal residual (GMRES) method [23] for solving the preconditioned least squares problems (AB-GMRES and BA-GMRES methods, respectively). For ill-conditioned problems, the AB-GMRES and BA-GMRES were shown to be more robust compared to the preconditioned CGNE and CGLS, respectively. Note here that the BA-GMRES works with Krylov subspaces in $n$-dimensional space, whereas the AB-GMRES works with Krylov subspaces in $m$-dimensional space. Since $m < n$ in the underdetermined case, the AB-GMRES works in a smaller dimensional space than the BA-GMRES and should be more computationally efficient compared to the BA-GMRES for each iteration. Moreover, the AB-GMRES has the advantage that the weight of the norm in (1) does not change for arbitrary $B$. Thus, we mainly focus on using the AB-GMRES to solve the underdetermined least squares problem (1). Morikuni [15] showed that the AB-GMRES may fail to converge to a least squares solution in finite-precision arithmetic for inconsistent problems. We will review this phenomenon. The GMRES applied to inconsistent problems was also studied in other papers [4, 5, 21, 16, 17].

In this paper, we first analyze the deterioration of convergence of the AB-GMRES. To overcome the deterioration, we use the normal equations of the upper triangular matrix arising in the AB-GMRES to change the inconsistent subproblem to a consistent one. In finite precision arithmetic, forming the normal equations for the subproblem will not square its condition number as would be predicted by theory. In the ill-conditioned case, the tiny singular values are shifted upwards due to rounding errors. In finite precision arithmetic, applying the standard Cholesky decomposition to the normal equations will result in a well-conditioned lower triangular matrix, which will ensure that the forward and backward substitutions work stably, and overcome the problem. Numerical experiments on a series of ill-conditioned Maragal matrices [6] show that the proposed method converges to a more accurate approximation than the original AB-GMRES. The method can also be used to solve general inconsistent singular systems.

The rest of the paper is organized as follows. In Section 2, we briefly review the AB-GMRES and the CGLS. In Section 3, we demonstrate and analyze the deterioration of the convergence. In Section 4, we propose and present a stabilized GMRES method and explain a regularization effect of the method based on the normal equations for ill-conditioned problems. In Section 5, numerical results for the underdetermined case and the square case are presented. In Section 6, we conclude the paper.

All the experiments in this paper were done using MATLAB R2017b in double precision, unless specified otherwise (where we extended the arithmetic precision by using the Multiprecision Computing Toolbox for MATLAB [1]), and the computer used was Alienware 15 CAAA15404JP with CPU Inter(R) Core(TM) i7-7820HK (2.90GHz).

2 Deterioration of convergence of AB-GMRES for inconsistent problems

In this section, we review previous results. First, we introduce the right-preconditioned GMRES (AB-GMRES), which is the basic algorithm in this paper. Then, we show the phenomenon that the convergence of the AB-GMRES deteriorates for inconsistent problems. Finally, we cite a related theorem to analyze the deterioration.

2.1 AB-GMRES method

The AB-GMRES method of Hayami et al. [10] applies the GMRES method [23] to

$$\min_{u \in \mathbb{R}^m} \|b - ABu\|_2, \quad x = Bu,$$

where $B \in \mathbb{R}^{n \times m}$.

Note the following.

Theorem 1. (Theorem 3.1 of [10])
Theorem 4. \( AB-GMRES \) exists (Lemma 3.3 of [10]) and hence \( R_i \striped{13} \) for

\[ \min_{x \in \mathbb{R}^n} \| b - Ax \|_2 = \min_{u \in \mathbb{R}^m} \| b - ABu \|_2 \]

holds for all \( b \in \mathbb{R}^m \) if and only if \( \mathcal{R}(A) = \mathcal{R}(AB) \).

Lemma 2. (Lemma 3.3 of [10]) \( \mathcal{R}(A^T) = \mathcal{R}(B) \Rightarrow \mathcal{R}(A) = \mathcal{R}(AB) \).

Theorem 3. (Theorem 3.6 of [10]) If \( \mathcal{R}(A^T) = \mathcal{R}(B) \), then \( \mathcal{R}(AB) = \mathcal{R}(B^T A^T) \iff \mathcal{R}(A) = \mathcal{R}(B^T) \).

Theorem 4. (Theorem 3.7 of [10]) If \( \mathcal{R}(A^T) = \mathcal{R}(B) \), then \( AB-GMRES \) determines a least squares solution of \( \min_{x \in \mathbb{R}^n} \| b - Ax \|_2 \) for all \( b \in \mathbb{R}^m \) and for all \( x_0 \in \mathbb{R}^n \) if and only if \( \mathcal{R}(A) = \mathcal{R}(B^T) \).

Let \( r = b - Ax = b - ABu \). Note

\[ \| r \|_2^2 = \| r \|_{\mathcal{R}(A)}^2 + \| r \|_{\mathcal{R}(A)\perp}^2 = \| r \|_{\mathcal{R}(A)}^2 + \| b \|_{\mathcal{R}(A)\perp}^2. \]

(6)

Here \( S^\perp \) denotes the orthogonal complement of subspace \( S \), and \( r_{\mathcal{R}(A)\perp} \) is the \( \mathcal{R}(A) \) component of \( r \), and \( r_{\mathcal{R}(A)\perp} \) is the \( \mathcal{R}(A) \perp \) (inconsistent) component of the residual vector \( r \). Thus, \( AB-GMRES \) minimizes \( \| r \|_2^2 \), and hence \( \| r \|_{\mathcal{R}(A)}^2 \).

The \( k \)-th iterate \( x_k \) is given by

\[ x_k = x_0 + Bu_k, \]

(7)

where \( u_k \in K_k(AB, r_0) = \text{span}\{ r_0, ABr_0, \ldots, (AB)^{k-1} r_0 \} \), so that \( x_k = x_0 + z_k \), where \( z_k \in K_k(BA, Br_0) = \text{span}\{ Br_0, (BA)Br_0, \ldots, (BA)^{k-1} Br_0 \} \).

Hence, if \( x_0 \in \mathcal{R}(B) \), \( x_k = v_k \in \mathcal{R}(B) \).

If, we let \( \mathcal{R}(B) = \mathcal{R}(A^T) \), then \( x_k \in \mathcal{R}(A^T) = \mathcal{N}(A)^\perp \). Further, if we let \( \mathcal{R}(B^T) = \mathcal{R}(A) \), then \( AB-GMRES \) will determine a least squares solution \( x_k \) (i.e. \( r_k|_{\mathcal{R}(A)} = 0 \)) where \( r_k = b - Ax_k \), and that solution \( x_k \) is a minimum-norm solution, since \( x_k \in \mathcal{N}(A)^\perp \).

The algorithm is given in Algorithm 1[10]. Here, \( H_{i+1,i} = (h_{pq}) \in \mathbb{R}^{(i+1)\times i} \) and \( e_1 = (1, 0, \ldots, 0)^T \in \mathbb{R}^{i+1} \).

| Algorithm 1 AB-GMRES |
|-----------------------|
| 1: Choose \( x_0 \in \mathbb{R}^n \), \( r_0 = b - Ax_0 \), \( v_1 = r_0/\| r_0 \|_2 \) |
| 2: for \( i = 1, 2, \ldots, k \) do |
| 3: \( u_i = ABv_i \) |
| 4: for \( j = 1, 2, \ldots, i \) do |
| 5: \( h_{i,j} = u_i^T v_j \), \( u_i = u_i - h_{i,j} v_j \) |
| 6: end for |
| 7: \( h_{i+1,i} = \| u_i \|_2 \), \( v_{i+1} = u_i/h_{i+1,i} \) |
| 8: Compute \( y_i \in \mathbb{R}^i \) which minimizes \( \| r_i \|_2 = \| r_0 \|_2 e_1 - H_{i+1,i} y_i \|_2 \) |
| 9: \( x_i = x_0 + B(v_1, v_2, \ldots, v_i) y_i \), \( r_i = b - Ax_i \) |
| 10: if \( \| A^T r_i \|_2 < \epsilon \| A^T r_0 \|_2 \) then |
| 11: \( \) stop |
| 12: \( \) end if |
| 13: end for |

To find \( y_i \in \mathbb{R}^i \) that minimizes \( \| r_i \|_2 = \| r_0 \|_2 e_1 - H_{i+1,i} y_i \|_2 \) in Algorithm 1 the standard approach computes the QR decomposition of \( H_{i+1,i} \)

\[ H_{i+1,i} = Q_{i+1} R_{i+1,i}, Q_{i+1} \in \mathbb{R}^{(i+1)\times (i+1)}, R_{i+1,i} = \begin{pmatrix} R_i & 0 \end{pmatrix} \in \mathbb{R}^{(i+1)\times i}, R_i \in \mathbb{R}^{i\times i}, \]

(8)

where \( Q_{i+1} \) is an orthogonal matrix and \( R_i \) is an upper triangular matrix. Then, backward substitution is used to solve a system with the coefficient matrix \( R_i \) as follows
Table 1: Information on the Maragal matrices.

| matrix       | m  | n  | density [%] | rank | $\kappa_2(A)$  |
|--------------|----|----|-------------|------|----------------|
| Maragal3T    | 858| 1682| 1.27        | 613  | $1.10 \times 10^3$ |
| Maragal4T    | 1027| 1964| 1.32        | 801  | $9.33 \times 10^6$ |
| Maragal5T    | 3296| 4654| 0.61        | 2147 | $1.19 \times 10^5$ |
| Maragal6T    | 10144| 21251| 0.25        | 8331 | $2.91 \times 10^6$ |
| Maragal7T    | 26525| 46845| 0.10        | 20843| $8.91 \times 10^6$ |

\[
\|r_i\|_2 = \min_{y_i \in \mathbb{R}^i} \|Q^T_{i+1} \beta e_1 - R_{i+1,i} y_i\|_2,
\]

where

\[
\beta = \|r_0\|_2, \quad Q^T_{i+1} \beta e_1 = \begin{pmatrix} t_i \\ \rho_{i+1} \end{pmatrix}, \quad t_i \in \mathbb{R}^i, \quad \rho_{i+1} \in \mathbb{R}, \quad y_i = R_{i+1}^{-1} t_i,
\]

\[
x_i = V_i y_i = V_i (R_i^{-1} t_i), \quad V_i = [v_1, v_2, \ldots, v_i] \in \mathbb{R}^{n \times i}, \quad V_i^T V_i = I,
\]

where $I$ is the identity matrix.

Here, Algorithm 4 is said to break down when $h_{i+1,i} = 0$. See Appendix B of [16].

From now on, we use AB-GMRES to solve (1) with $B = A^T$ and $x_0 \in \mathcal{R}(A^T)$, e.g. $x_0 = 0$, which means $x_k = x_0 + z_k$, where $z_k \in \mathcal{K}(A^T A, A^T r_0)$. Hence, Theorem 2 guarantees the convergence in exact arithmetic even in the inconsistent case. Note also that the AB-GMRES is mathematically equivalent to CGLS with $x_0 \in \mathcal{R}(A^T)$, although the behaviour in finite precision arithmetic may be different. (See section 2.2.) Moreover, in finite precision arithmetic, AB-GMRES may fail to converge to a least squares solution for inconsistent problems, as shown later.

2.2 The CGLS method

The CGLS (CNRG) method [11, 22] applies the conjugate gradient (CG) method [11] to the normal equations of the first kind [3]. CGLS minimizes

\[
(e, A^T A e) = \|r|_{\mathcal{R}(A)}\|_2^2,
\]

where $e = x - x^*$, where $x^*$ is any solution of (3), and $r|_{\mathcal{R}(A)}$ is the $\mathcal{R}(A)$ component of $r = b - Ax$ and the $k$-th iterate is given by

\[
x_k = x_0 + z_k
\]

where

\[
z_k \in \mathcal{K}(A^T A, A^T r_0) = \text{span} \{A^T r_0, (A^T A)A^T r_0, \ldots, (A^T A)^{k-1} A^T r_0\},
\]

where $r_0 = b - Ax_0$.

Thus, if $x_0 \in \mathcal{R}(A^T)$, e.g. $x_0 = 0$, then $x_k \in \mathcal{R}(A^T) = \mathcal{N}(A)^\perp$. Therefore, when CGLS converges, it converges to the minimum-norm least squares solution $A^T b$. (See e.g. [2], p.291.) However, in finite precision arithmetic, CGLS may not converge well as in exact arithmetic, and may require reorthogonalization [10] or preconditioning, especially when the problem is ill-conditioned.

2.3 AB-GMRES for inconsistent problems

In this section, we perform experiments to show that the convergence of AB-GMRES deteriorates for inconsistent problems. Experiments were done on the transpose of the matrix Maragal3T, denoted by Maragal3T etc. Table 1 gives the information on the Maragal matrices, including the density of nonzero entries, rank and condition number. Here, the rank and condition number were determined by using the MATLAB functions spnrank [3] and svd, respectively.
Figure 1 shows the relative residual norm $\|A^T r_i\|_2 / \|A^T b\|_2$ and $\kappa_2(R_i)$ versus the number of iterations for AB-GMRES with $B = A^T$ for Maragal3T, where $r_i = b - A x_i$, and the vector $b$ was generated by the MATLAB function `rand` which returns a vector whose entries are uniformly distributed in the interval (0, 1). Therefore generically $b \not\in R(A)$ and the problem is inconsistent. Here $\kappa_2(R_i) = \kappa_2(B_{i+1,l})$ holds from (8). The value of $\kappa_2(R_i)$ was computed by the MATLAB function `cond`. The relative residual norm $\|A^T r_i\|_2 / \|A^T b\|_2$ decreased to $10^{-8}$ until the 525th iteration, and then increased sharply. The value of $\kappa(R_i)$ started to increase rapidly around iterations 450–550. This observation shows that $R_i$ becomes ill-conditioned before convergence. Thus, AB-GMRES failed to converge to a least squares solution. This phenomenon was observed by Morikuni [15].

The reason why $R_i$ becomes ill-conditioned before convergence in the inconsistent case will be explained by a theorem in the next subsection.

### 2.4 GMRES for inconsistent problems

Brown and Walker [4] introduced an effective condition number to explain why GMRES fails to converge for inconsistent least squares problems

$$\min_{x \in \mathbb{R}^m} \|b - \tilde{A} x\|_2,$$

where $\tilde{A} \in \mathbb{R}^{m \times m}$ is singular, in the following Theorem 5.

Let $b|_{R(\tilde{A})}$ denote the orthogonal projection of $b$ onto $R(\tilde{A})$. Assume $\mathcal{N}(\tilde{A}) = \mathcal{N}(\tilde{A}^T)$ and $grade(\tilde{A}, b)$ for $\tilde{A} \in \mathbb{R}^{m \times m}$, $\tilde{b} \in \mathbb{R}^m$ is defined as the minimum $k$ such that $K_{k+1}(\tilde{A}, b) = K_k(\tilde{A}, b)$. Then, $\dim(K_k(\tilde{A}, b)|_{R(\tilde{A})}) = \dim(K_{k+1}(\tilde{A}, b)|_{R(\tilde{A})})$ is defined as the minimum $k$ such that $K_{k+1}(\tilde{A}, b) = K_k(\tilde{A}, b)$. Then, $\dim(K_k(\tilde{A}, b)|_{R(\tilde{A})}) = \dim(K_{k+1}(\tilde{A}, b)|_{R(\tilde{A})}) = k$ (See Appendix A). Since $\mathcal{N}(\tilde{A}) = \mathcal{N}(\tilde{A}^T)$, we obtain $\tilde{A} b|_{R(\tilde{A})} = \tilde{A} b$ and $\dim(K_{k+1}(\tilde{A}, b)) = \dim(K_{k+1}(\tilde{A}, b)|_{R(\tilde{A})}) = k$. If $b \not\in R(\tilde{A})$ and $\dim(K_{k+1}(\tilde{A}, b)) = k$, $\dim(K_{k+1}(\tilde{A}, b)|_{R(\tilde{A})}) = k + 1$ (See Appendix B).

Let $x_0$ be the initial solution and $r_0 = b - \tilde{A} x_0$. In the inconsistent case, a least squares solution is obtained at iteration $k$, and at iteration $k + 1$ breakdown occurs because of $\dim(K_{k+1}(\tilde{A}, r_0)) < \dim(K_{k+1}(\tilde{A}, r_0))$, i.e. rank deficiency of $\min_{z \in K_{k+1}(\tilde{A}, r_0)} \|b - \tilde{A}(x_0 + z)\|_2 = \min_{z \in K_{k+1}(\tilde{A}, r_0)} \|r_0 - A z\|_2$. This case is also called the hard breakdown [24].

However, even if $\mathcal{N}(\tilde{A}) = \mathcal{N}(\tilde{A}^T)$, when (15) is inconsistent, the least squares problem $\min_{z \in K_{k+1}(\tilde{A}, r_0)} \|r_0 - A z\|_2$ may become ill-conditioned as shown below.

**Theorem 5.** [4] Assume $\mathcal{N}(\tilde{A}) = \mathcal{N}(\tilde{A}^T)$, and denote the least squares residual of (15) by $r^*$, the residual at the $(i-1)$st iteration by $r_{i-1}$. If $r_{i-1} \neq r^*$, then

$$\kappa_2(A_i) \geq \frac{\|A_i\|_2 \|r_{i-1}\|_2}{\|A_i\|_2 \sqrt{\|r_{i-1}\|_2^2 - \|r^*\|_2^2}},$$

(16)
where \( A_i = \widetilde{A}_{|K_i(A,r_0)} \) and \( \bar{A}_i = \widetilde{A}_{|K_i(A,r_0)+\text{span}\{r^*\}} \). Here, \( \widetilde{A}|_S \) is the restriction of \( \widetilde{A} \) to a subspace \( S \subseteq \mathbb{R}^m \).

Theorem 5 implies that GMRES suffers ill-conditioning for \( b \not\in \mathcal{R}(\widetilde{A}) \) as \( \|r_i\| \) approaches \( \|r^*\| \). We can apply Theorem 5 to AB-GMRES for least-squares problems by setting \( \widetilde{A} \equiv AA^T \). Theorem 5 also implies that even if we choose \( B \) as \( A^T \), which satisfies the conditions in Theorem 4, AB-GMRES still may not converge numerically because of the ill-conditioning of \( R_i \), losing accuracy in the solution computed in finite-precision arithmetic when \( r_{i-1} \) approaches \( r^* \).

3 Analysis of the deterioration of convergence

In this section, we illustrate the deterioration of convergence of GMRES through numerical experiments. There are two points to note in this section. The first point is that the condition number of \( R_i \) tends to become very large as the iteration proceeds for inconsistent problems. Due to \( H_{i+1,i} = Q_{i+1}R_{i+1,i} \), the condition number of \( H_{i+1,i} \) is the same as that of \( R_i \), and will also become very large. The second point is as follows. Since \( y_i = R_i^{-1}t_i \), \( y_i \) is obtained by applying backward substitution to the triangular system \( R_i y_i = t_i \). When the triangular system becomes ill-conditioned, backward substitution becomes numerically unstable, and fails to give an accurate solution \( y_i \).

Figure 1 shows that at step 550 the relative residual norm suddenly increases. To understand this increase, observe the singular values of \( R_{550} \).

The left of Figure 2 shows the singular values of \( R_{550} \) which were computed in double precision arithmetic. The smallest singular value of \( R_{550} \) is \( 3.21 \times 10^{-14} \), which means that the triangular matrix \( R_{550} \) is very ill-conditioned and nearly singular in double precision arithmetic.

The right of Figure 2 shows the singular values of \( R_{550} \) which were computed in quadruple precision arithmetic using the Multiprecision Computing Toolbox for MATLAB. The smallest singular value of \( R_{550} \) is \( 5.39 \times 10^{-15} \). Since quadruple precision is more accurate, from now on, we mainly show singular value distributions computed in quadruple precision.

Figure 3 shows \( \kappa_2(R_i) \), \( \|y_i\|_2 \), and the relative residual norm \( \|t_i - R_i y_i\|_2 / \|t_i\|_2 \) versus the number of iterations for AB-GMRES. The relative residual norm increases only gradually when the condition number of \( R_i \) is less than \( 10^8 \). When the condition number of \( R_i \) becomes larger than \( 10^{10} \), the relative residual norm starts to increase sharply. This observation shows that when the condition number of \( R_i \) becomes very large, the backward substitution will fail to give an accurate \( y_i \). As a result, we would not get an accurate \( x_i \), and the convergence of AB-GMRES would deteriorate.

4 Stabilized GMRES method

In this section, we first propose and present a stabilized GMRES method. Then, we explain its regularization effect comparing it with other regularization techniques.
4.1 The stabilized GMRES

In order to overcome the deterioration of convergence of GMRES for inconsistent systems, we propose solving the normal equations

$$R_i^T R_i y_i = R_i^T t_i$$  \hspace{1cm} (17)

instead of $R_i y_i = t_i$, which we will call the stabilized GMRES. This makes the system consistent, and stabilizes the process, as will be shown in the following.

One may also consider using the normal equations of $H_{i+1,i}$. However, before breakdown, we use AB-GMRES, which means we do not have to store $H_{i+1,i}$. We only store $R_i$ and update it in each iteration, which is cheaper.

Figure 4 shows the relative residual norm $\|A^T r\|_2 / \|A^T r_0\|_2$ versus the number of iterations for the standard AB-GMRES and stabilized AB-GMRES with $B = A^T$ for Maragal3T. The stabilized method reaches the relative residual norm level of $10^{-11}$ which improves a lot compared to the standard method. The method which we used for solving the normal equations (17) is the standard Cholesky decomposition. We replace line 8 of Algorithm 1 by Algorithm 2.

We first checked that the method works for the standard Cholesky decomposition coded by ourselves. Later we applied the backslash function of Matlab to (17) to speed up. We checked that in the backslash, the Cholesky decomposition method chol is used until the GMRES residual norm stagnates at a small level as seen in Figure 4. In order to continue with further GMRES iterations, the chol is automatically switched to the ldiv, which works even for singular systems.

In spite of the above mentioned merits of stabilization, solving the normal equations in AB-GMRES is expensive. Actually, we only need the stabilized AB-GMRES when $R_i$ becomes ill-conditioned. Thus,
we can speed up the process by switching AB-GMRES to stabilized AB-GMRES only when $R_i$ becomes ill-conditioned. The condition number of an incrementally enlarging triangular matrix can be estimated by techniques in [24]. In this paper, we adopt the switching strategy by monitoring the relative residual norm $\|A^t r_i\|_2/\|A^t r_0\|_2$. Let $\text{ATR}(i) = \|A^t r_i\|_2/\|A^t r_0\|_2$ for the $i$th iteration. When $\text{ATR}(v)/ \min_{i=1,2,\ldots,v-1} \text{ATR}(i) > 10$, we judge that a jump in relative residual norm has occurred, and we switch AB-GMRES to stabilized AB-GMRES at the $v$th iteration.

Motivated by the stabilized AB-GMRES, we also applied the truncated singular value decomposition (TSVD) stabilization method and compared it with the stabilized AB-GMRES. The method modifies $R_i$ by truncating singular values smaller than $\mu$. More specifically, let $R_i = U \Sigma V^T$ be the SVD of $R_i$, where the columns of $U = [u_1, u_2, \ldots, u_i]$ and $V = [v_1, v_2, \ldots, v_i]$ are the left and right singular vectors, respectively, and the diagonal entries of $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_i)$ are the singular values of $R_i$ in descending order $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_i$. Then, the TSVD approximates $R_i \simeq \sum_{j=1}^k \sigma_j u_j v_j^T$ with $k$ such that $\sigma_{k+1} \leq \mu \sigma_1 \leq \sigma_k$ and $y_i = R_i^{-1} t_i \simeq \sum_{j=1}^k \frac{1}{\sigma_j} v_j u_j^T t_i$.

When $\mu = 10^{-13}, 10^{-12}, \ldots, 10^{-4}$, the method converges but when $\mu$ is smaller than $10^{-13}$ or larger than $10^{-4}$, it diverges and is similar to the original AB-GMRES. Numerical experiments showed that $\mu = \sqrt{\epsilon} \simeq 10^{-8}$, where $\epsilon$ is the machine epsilon (about $10^{-16}$ in double precision arithmetic), gave the best result among $\mu = 10^{-4}, 10^{-2}, \ldots, 10^{-16}$ in terms of the relative residual as shown in Figure 4 for the problem Maragal3T. The convergence behaviour of the TSVD stabilization method is similar to the stabilized AB-GMRES method, which suggests that eliminating tiny singular values which are less than $10^{-8}$ is effective for solving problem 4. However, the TSVD method requires computing the truncated singular value decomposition of $R_i$, and requires choosing the value of the threshold parameter $\mu$, whereas the stabilized AB-GMRES does not require either of them.

Table 2 gives more results for the Maragal matrices. The table shows that the stabilized AB-GMRES is more accurate than the standard AB-GMRES. This seems paradoxical, since forming the normal equations whose coefficient matrix $A^T R_i$ would square the condition number compared to $R_i$, which would make the ill-conditioned problem even worse. Why can the stabilized AB-GMRES give a more accurate solution? We will explain why the stabilized AB-GMRES works in the next subsection.

### 4.2 Why the stabilized GMRES method works

Consider solving $R_i y_i = t_i$, $R_i \in \mathbb{R}^{i \times i}$, $t_i \in \mathbb{R}^i$ by solving the normal equations [47], which, in theory, squares the condition number and makes the problem become harder to solve numerically. However, in finite precision arithmetic, the condition number of the normal equations is not necessarily squared. We will continue to illustrate the phenomenon by using the example in Section 3.
We used the MATLAB function \texttt{svd} in quadruple precision arithmetic \cite{1} to calculate the singular values. The smallest singular value of $R_{550}$ is $5.39 \times 10^{-15}$, so its square is $2.91 \times 10^{-29}$.

Let $\text{fl}(\cdot)$ denote the evaluation of an expression in floating point arithmetic and $\text{fl}_d(\cdot)$ and $\text{fl}_q(\cdot)$ denote the result in double precision arithmetic and quadruple precision arithmetic, respectively. Figure 5 shows that, numerically, the smallest singular value of $\text{fl}_d(R_{550}^T R_{550})$ is $7.21 \times 10^{-14}$, which is much larger than $2.91 \times 10^{-29}$. Further, the Cholesky factor $L$ of $\text{fl}_d(R_{550}^T R_{550}) = LL^T$ computed in double precision precision arithmetic has the smallest singular value $3.50 \times 10^{-7}$, which is also larger than $\sqrt{2.91 \times 10^{-29}} = 5.39 \times 10^{-15}$. Thus, the triangular systems $Lz_i = \tilde{t}_i$ and $L^T y_i = z_i$ are better-conditioned than $R_i y_i = t_i$, which will ensure the stability of the forward and backward substitutions and succeeds in obtaining a much more accurate solution than the standard approach.

The left of Figure 6 compares the singular values $\sigma_i(\text{fl}_d(R_{550}^T R_{550}))$, $\sigma_i(R_{550})^2$, $\sigma_i(\text{fl}_d(R_{610}^T R_{610}))$, and $\sigma_i(R_{610})^2$ in quadruple precision arithmetic.

Experiment results show that finite precision arithmetic has the effect of shifting the tiny singular value upwards. That is the reason why the normal equations (17) help to reduce the condition number and makes the problem become better-conditioned.

Next, we computed the multiplication $R_{550}^T R_{550}$ in quadruple precision arithmetic and observed that the smallest singular values of $R_{550}^T R_{550}$ coincided with the squared singular values $\sigma_i(R_{550})^2$ (blue circle...
symbol) in the left of Figure 6, unlike in double precision computation. Since the maximum of the elements of $\hat{f}_d(R_{550}^T R_{550}) - \hat{f}_d(R_{550}^T R_{550})$ is approximately $8.16 \times 10^{-12}$, double precision arithmetic contains error of the order of $10^{-12}$. Thus, double precision arithmetic has an effect of regularizing the matrix $R_{550}^T R_{550}$, since double precision matrix multiplication is not accurate enough to keep all the information.

4.3 Quadruple precision

In order to see the effect of the machine precision $\epsilon$ on the convergence of the AB-GMRES, we compared the stabilized AB-GMRES with the AB-GMRES in quadruple precision arithmetic for the problem Maragal 3T in Figure 7. For both methods, the relative residual norm reached a smaller level of $10^{-16}$ compared to $10^{-12}$ and $10^{-8}$, respectively, for double precision arithmetic in Figure 4. The curve of the relative residual norm became smoother compared to double precision. As seen in Figure 7, the relative residual norm of the stabilized GMRES method jumped to $10^{-1}$ after reaching $10^{-16}$, whereas the relative residual norm of the AB-GMRES method stayed around $10^{-16}$.

4.4 When the stabilized GMRES method works

Motivated by the Läuchli matrix [12], we consider solving the following EP (equal projection) problem

$$A_3 x = \begin{pmatrix} 1 \sqrt{2} \sqrt{2} \epsilon \sqrt{6} \sqrt{6} \\ 1 \sqrt{2} \sqrt{2} \epsilon \sqrt{6} \\ 0 0 1 \end{pmatrix} x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

(18)

where $\epsilon$ is the machine epsilon.

Apply GMRES with $x_0 = 0$ to (18). Let $R_s \in \mathbb{R}^{s \times s}$ be the upper triangular matrix obtained at the $s$th iteration of GMRES. In the second iteration, after applying the Givens rotation to $H_{3,2}$, we obtain the following:

$$R_2 = \begin{pmatrix} 1 & 1 \\ 0 & \sqrt{\epsilon} \end{pmatrix}, \quad R_2^T R_2 = \begin{pmatrix} 1 & 1 & 1 + \epsilon \\ 1 & 1 \\ 1 & 1 \end{pmatrix} \simeq \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

(19)

Thus, there is a risk that the stabilized GMRES will give a numerically singular matrix $R_2^T R_2$ in finite precision arithmetic for nonsingular $R_2$. We will analyze this phenomenon.

We define the following.
\[ O(\epsilon) \text{ denotes that there exists a constant } c \text{ independent of } \epsilon, \text{ such that } -c\epsilon < O(\epsilon) < c\epsilon. \] Also, let

\[ O(\epsilon) = \begin{pmatrix} O(\epsilon) \\ O(\epsilon) \\ \vdots \\ O(\epsilon) \end{pmatrix} \in \mathbb{R}^n, \quad O(\epsilon) = [O(\epsilon), O(\epsilon), \ldots, O(\epsilon)] \in \mathbb{R}^{n \times n}. \quad (20) \]

We assume that the basic arithmetic operations \( op = +, -, \ast, / \) satisfy \( \text{fl}(x \ op \ y) = (x \ op \ y)(1 + O(\epsilon)) \) as in [13].

Note also that the following theorem holds from Theorem 8.10 of [13]. Let \( x, y \in \mathbb{R}^n, A, B \in \mathbb{R}^{n \times n}, \) and

\[
|x| = \begin{pmatrix} |x_1| \\ |x_2| \\ \vdots \\ |x_n| \end{pmatrix} \quad \text{for} \quad x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad (21)
\]

\[
|A| = \begin{pmatrix} |a_{11}| & |a_{12}| & \cdots & |a_{1n}| \\ |a_{21}| & |a_{22}| & \cdots & |a_{2n}| \\ \vdots & \vdots & \ddots & \vdots \\ |a_{n1}| & |a_{n2}| & \cdots & |a_{nn}| \end{pmatrix} \quad (22)
\]

for \( A = (a_{pq}) \). Then

\[
\text{fl}(x^T y) = x^T y + O(\epsilon)|x|^T|y| = x^T y + O(\epsilon),
\]

\[
\text{fl}(Ax) = Ax + O(\epsilon)|A||x| = Ax + O(\epsilon),
\]

\[
\text{fl}(AB) = AB + O(\epsilon)|A||B| = AB + O(\epsilon).
\]

Note also that the following theorem holds from Theorem 8.10 of [13].

**Theorem 6.** Let \( T = (t_{pq}) \in \mathbb{R}^{n \times n} \) be a triangular matrix and \( b \in \mathbb{R}^n \). Then, the computed solution \( \hat{x} \) obtained from substitution applied to \( Tx = b \) satisfies

\[
\hat{x} = x + O(n^2 \epsilon)M(T)^{-1}|b|. \quad (23)
\]

Here, \( M(T) = (m_{ij}) \) is the comparison matrix such that

\[
m_{ij} = \begin{cases} |t_{ij}|, & i = j, \\ -|t_{ij}|, & i \neq j. \end{cases} \quad (24)
\]

Further, we define the following.

Assume \( \|A\|_2 = O(1) \). We say \( A \in \mathbb{R}^{n \times n} \) is numerically nonsingular if and only if

\[
\text{fl}(Ax) = O(\epsilon) \quad \Rightarrow \quad x = O(\epsilon). \quad (25)
\]

Note that this definition of numerical nonsingularity agrees with that of numerical rank due to the following.

Let the SVD of \( A = U\Sigma V^T \) where \( U, V \) are orthogonal matrices and \( \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n) \). Here, \( \|A\|_2 = \sigma_1 = O(1) \). If the numerical rank of \( A \) is \( r < n \), there is a \( \sigma_i = O(\epsilon), \ r + 1 \leq i \leq n \). Then, \( Ax = U\Sigma V^T x = O(\epsilon) \) admits \( x' = V^T x = (x'_1, x'_2, \ldots, x'_n)^T \) such that \( x'_i = O(1) \), and hence \( x = O(1) \). Thus, \( A \) is numerical singular. Then, the following theorem holds.
Theorem 7. Let $R_s = (r_{pq}) \in \mathbb{R}^{s \times s}$ be an upper-triangular matrix and

\[
R_{s+1} = \begin{pmatrix} R_s & d \\ 0 & r_{s+1,s+1} \end{pmatrix} \in \mathbb{R}^{(s+1) \times (s+1)}.
\] (26)

Assume $R_s$ is numerically nonsingular, and $R_s = O(1), R_s^{-1} = O(1), M(R_s)^{-1} = O(1)$, $d = O(1)$ and $O(s) = O(s^2) = O(1)$. Then, the following holds:

\[ \Phi(R_s^T R_{s+1}) \text{ is numerically nonsingular } \iff \Phi(r_{s+1,s+1}^2) > \Phi(d^T d) O(\epsilon). \]

Proof. See Appendix C. □

Theorem 7 gives the necessary and sufficient condition so that the stabilized GMRES works the $(s+1)$st iteration, i.e., $R_{s+1}^T R_{s+1}$ is numerically nonsingular.

The difficulty in solving $R_i y_i = t_i$ by backward substitution is not because the diagonals of $R_i$ are tiny. The reason is that $R_i$ has tiny singular values. However, the exceptional example (19) exists where the stabilized AB-GMRES does not work. The condition $\Phi(r_{s+1,s+1}^2) > \Phi(d^T d) O(\epsilon)$ in Theorem 7 excludes such exceptions.

Figure 8 shows $r_{s+1,s+1}^2$ and $d^T d$ together with the convergence of the AB-GMRES and that of the stabilized AB-GMRES for Maragal_3T. The figure shows that up to 613 iterations, the conditions in Theorem 7 are satisfied, and $R_{s+1}^T R_{s+1}$ is numerically nonsingular, so that the stabilized AB-GMRES works.

### 4.5 Comparison with Tikhonov regularization method

Another approach to stabilize the AB-GMRES would be to apply Tikhonov regularization. There are two methods to implement it. The first method is to solve the following square system:

\[
(R_i^T R_i + \lambda I) y_i = R_i^T t_i, \quad \lambda \geq 0
\] (27)

using the Cholesky decomposition.

The second method is to solve the regularized least squares problem

\[
\min_{y_i \in \mathbb{R}^n} \left\| \begin{pmatrix} t_i \\ 0 \end{pmatrix} - \begin{pmatrix} R_i \\ \sqrt{\lambda} I \end{pmatrix} y_i \right\|_2
\] (28)

using the QR decomposition.

These two methods are equivalent mathematically. However, they are not equivalent numerically. The behavior of the first method is similar to the stabilized AB-GMRES. Table 3 shows that AB-GMRES combined with the first method converges better when $\lambda = 10^{-16}$ than when $\lambda = 10^{-14}$. This method
can be used to shift upwards the small singular values, but is less accurate compared to the stabilized AB-GMRES (cf. Table 2).

Table 3 also shows that the second method is even more accurate compared with the stabilized AB-GMRES method. There is no need to form the normal equations, so that less information is lost due to rounding error. However, one needs to choose an appropriate value for the regularization parameter \( \lambda \). Figure 9 shows the relative residual norm \( \frac{\| \mathbf{A}^T \mathbf{r}_i \|_2}{\| \mathbf{A}^T \mathbf{r}_0 \|_2} \) for the regularized AB-GMRES using (28) versus the number of iterations for different values of \( \lambda \) for Maragal3T. According to Figure 9, \( \lambda = 10^{-16} \) was optimal among \( 10^{-12}, 10^{-14}, 10^{-16}, 10^{-18} \), so we recommend this value in practice.

We here note the following.

**Theorem 8.** Let \( \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_i \) be the the singular values of \( \mathbf{R}_i \). Then, the singular values of \( \mathbf{R}_i' = \left( \mathbf{R}_i \sqrt{\lambda \mathbf{I}} \right) \) are given by \( \sqrt{\sigma_1^2 + \lambda} \geq \sqrt{\sigma_2^2 + \lambda} \geq \cdots \geq \sqrt{\sigma_i^2 + \lambda} \).

**Proof.** See Appendix D.

Then, let
\[
\kappa \equiv \kappa_2(\mathbf{R}_i) = \frac{\sigma_1}{\sigma_i}, \quad \kappa^2 \equiv \kappa_2(\mathbf{R}_i')^2 = \frac{\sigma_1^2 + \lambda}{\sigma_1^2/\kappa^2 + \lambda} = 1 + \frac{\sigma_1^2(1 - 1/\kappa^2)}{\sigma_1^2/\kappa^2 + \lambda}. \tag{30}
\]

Since \( \kappa \geq 1, \, \text{d} \kappa^2/\text{d} \lambda \leq 0 \) for \( \lambda \geq 0 \) and \( \kappa^2(\lambda = 0) = \kappa, \, \kappa^2(\lambda = +\infty) = 1 \). Note also that
\[
\lambda = \frac{\sigma_1^2[1 + (\kappa^2/\kappa^2)]}{\kappa^2 - 1}. \tag{31}
\]

Therefore, for instance, if \( \kappa \gg 1 \) and we want \( \kappa' = \sqrt{\kappa} \),
\[
\lambda = \frac{\sigma_1^2(1 + 1/\kappa)}{\kappa - 1} \simeq \frac{\sigma_1^2}{\kappa}. \tag{32}
\]

For example, if \( \kappa = 10^{16} \) and we want \( \kappa' = 10^8 \), we should choose \( \lambda \simeq \sigma_1^2 \times 10^{-16} \). For Maragal3T, the largest singular value \( \sigma_1 \) is about 12.64, so that we can estimate a reasonable value of \( \lambda \simeq 1.60 \times 10^{-14} \). However, this estimation assumes \( \kappa' = \sqrt{\kappa} \), and needs an extra cost for computing \( \sigma_1 \). See [3] for other estimation techniques for the regularization parameter.
Table 3: Attainable smallest relative residual norm $\|A^T r_i\|_2/\|A^T r_0\|_2$ for AB-GMRES with Tikhonov regularization using (27) and (28).

| matrix          | Maragal_3T | Maragal_4T | Maragal_5T | Maragal_6T | Maragal_7T |
|-----------------|------------|------------|------------|------------|------------|
| iter. method    | 552        | 597        | 1304       | 2440       | 1864       |
| $\lambda = 10^{-14}$ | $5.08 \times 10^{-11}$ | $5.57 \times 10^{-8}$ | $1.05 \times 10^{-5}$ | $8.26 \times 10^{-6}$ | $4.53 \times 10^{-6}$ |
| iter. method    | 570        | 598        | 1226       | 2440       | 1864       |
| $\lambda = 10^{-16}$ | $5.80 \times 10^{-12}$ | $5.59 \times 10^{-8}$ | $4.22 \times 10^{-6}$ | $8.26 \times 10^{-6}$ | $4.53 \times 10^{-6}$ |
| method (28) $\lambda = 1.6 \times 10^{-14}$ | 553        | 547        | 1261       | 2937       | 2475       |
| iter.           | 551        | 547        | 1262       | 3037       | 2475       |
| $\lambda = 10^{-16}$ | $3.37 \times 10^{-12}$ | $5.59 \times 10^{-8}$ | $5.64 \times 10^{-7}$ | $1.91 \times 10^{-6}$ | $2.78 \times 10^{-7}$ |

Table 4: Comparison of the attainable smallest relative residual norm $\|A^T r_i\|_2/\|A^T r_0\|_2$.

| matrix         | Maragal_3T | Maragal_4T | Maragal_5T | Maragal_6T | Maragal_7T |
|----------------|------------|------------|------------|------------|------------|
| iter.          | 531        | 465        | 1110       | 2440       | 1864       |
| standard AB-GMRES | $1.05 \times 10^{-8}$ | $2.09 \times 10^{-7}$ | $5.35 \times 10^{-6}$ | $8.26 \times 10^{-6}$ | $4.53 \times 10^{-6}$ |
| iter.          | 552        | 598        | 1226       | 3002       | 2459       |
| stabilized AB-GMRES | $5.99 \times 10^{-12}$ | $5.59 \times 10^{-8}$ | $4.22 \times 10^{-6}$ | $3.88 \times 10^{-6}$ | $2.80 \times 10^{-7}$ |
| iter.          | 553        | 565        | 1223       | 2374       | 2474       |
| RR-AB-GMRES    | $2.57 \times 10^{-11}$ | $5.59 \times 10^{-8}$ | $3.62 \times 10^{-6}$ | $1.63 \times 10^{-5}$ | $2.78 \times 10^{-7}$ |
| iter.          | 562        | 626        | 1263       | 4373       | 5658       |
| BA-GMRES       | $2.88 \times 10^{-14}$ | $7.92 \times 10^{-11}$ | $2.29 \times 10^{-12}$ | $5.12 \times 10^{-11}$ | $2.03 \times 10^{-10}$ |
| iter.          | 1682       | 2375       | 4576       | 151013     | 97348      |
| LSQR           | $5.64 \times 10^{-14}$ | $2.77 \times 10^{-10}$ | $1.11 \times 10^{-11}$ | $5.87 \times 10^{-10}$ | $1.33 \times 10^{-9}$ |
| iter.          | 1654       | 2308       | 4273       | 127450     | 70242      |
| LSMR           | $5.51 \times 10^{-14}$ | $3.00 \times 10^{-10}$ | $3.25 \times 10^{-11}$ | $4.16 \times 10^{-10}$ | $9.95 \times 10^{-10}$ |

5 **Comparisons with other methods**

We show the numerical performance of the proposed stabilized AB-GMRES method on test matrices, compared with previous methods. All programs for iterative methods were coded according to the algorithms in [18, 19, 20, 21]. Each method was terminated at the iteration step which gives the minimum relative residual norm within m iterations, where m is the number of the rows of the matrix. No restarts were used for GMRES. Experiments were done for rank-deficient matrices whose information is given in Table 1. Here, we have deleted the zero rows and columns of the test matrices beforehand. The elements of $b$ were randomly generated using the MATLAB function `rand`. Therefore generically $b \not\in \mathcal{R}(A)$ and the problem is inconsistent. Each experiment was done 10 times for the same right hand side $b$ and the average of the CPU times are shown. Symbol - denotes that $\|A^T r_i\|_2/\|A^T r_0\|_2$ did not reach $10^{-8}$ within 20 iterations.

5.1 **Underdetermined inconsistent least squares problems**

First, we compared the proposed stabilized AB-GMRES with the range restricted AB-GMRES (RR-AB-GMRES) [18], where the Krylov subspace for the RR-AB-GMRES with $B = A^T$ is $K_r(A^T, AA^T r_0)$, AB-GMRES with $B = A^T$, BA-GMRES with $B = A^T$, LSQR [20] and LSMR [21].

Table 4 shows that the stabilized AB-GMRES is generally more accurate than the RR-AB-GMRES. The
Table 5: Comparison of the CPU time (seconds) to obtain relative residual norm $\|A^T r_i\|_2 / \|A^T r_0\|_2 < 10^{-8}$.

| matrix | Maragal_3T | Maragal_4T | Maragal_5T | Maragal_6T | Maragal_7T |
|--------|------------|------------|------------|------------|------------|
| iter.  | -          | -          | -          | -          | -          |
| standard AB-GMRES | - | - | - | - | - |
| iter.  | 546 (526)  | -          | -          | -          | -          |
| stabilized AB-GMRES | 2.01 | - | - | - | - |
| RR-AB-GMRES | 1.84 | - | - | - | - |
| iter.  | 545        | -          | -          | -          | -          |
| BA-GMRES | 2.10 | 3.19 | $4.25 \times 10^1$ | $1.81 \times 10^3$ | 9.20 $\times 10^3$ |
| iter.  | 530        | 608        | 1232       | 3623       | 5001       |
| LSQR | $1.27 \times 10^{-1}$ | $2.56 \times 10^{-1}$ | 1.49 | $2.93 \times 10^2$ | $4.33 \times 10^2$ |
| iter.  | 1456       | 1989       | 4013       | 54017      | 31206      |
| LSMR | $1.25 \times 10^{-1}$ | $2.37 \times 10^{-1}$ | 1.49 | $1.50 \times 10^2$ | $2.23 \times 10^2$ |

Figure 10: Relative error for CGLS, AB-GMRES and stabilized AB-GMRES for Maragal_3T ($\epsilon = 0.01$).

5.2 Comparison with CGLS

Next, we compare the stabilized AB-GMRES (with $B = A^T$, $x_0 = 0$) with CGLS (with $x_0 = 0$) and AB-GMRES (with $B = A^T$, $x_0 = 0$), which are all mathematically equivalent in the sense that they all minimize $\|r\|_{\mathcal{R}(A)}$, generate approximate solutions $x_k \in x_0 + K_k(A^T A, A^T r_0)$, and converge to the minimum-norm solution of (1). We test the methods for inconsistent $b$ containing noise as follows. Given $x' \in \mathbb{R}^n$, compute $b' = (b'_1, b'_2, \ldots, b'_m)^T = A x' \in \mathcal{R}(A)$, and let $b = (b_1, \ldots, b_m)^T$, where $b_i = b'_i \{1 + (−1 + 2u_i)\epsilon\}$. $u_i$ is a uniform random number in the interval $[0, 1]$, $1 \leq i \leq m$, and $\epsilon = 0.01, 0.1, 0.2, 0.5$. Then, we compare $\|x_k - x^*\|_2 / \|x^*\|_2$ for each method where $x^* = A^T b$ is computed by using the truncated SVD (in quadruple precision arithmetic).

The Figure 10 show the case when $\epsilon = 0.01, 0.1, 0.2, 0.5$, respectively, where $\|b\|_{\mathcal{R}(A)} / \|b\|_2 \approx 0.002, 0.02, 0.04, 0.12$ for Maragal_3T. The CGLS gave the most accurate minimum-norm solution, and both AB-GMRES and stabilized AB-GMRES converged to the minimum-norm solution. Stabilized AB-GMRES is better than AB-GMRES in the sense that it did not diverge and gave a solution with smaller error for
Figure 11: Relative error for CGLS, AB-GMRES and stabilized AB-GMRES for Maragal3T ($\epsilon = 0.1$).

Figure 12: Relative error for CGLS, AB-GMRES and stabilized AB-GMRES for Maragal3T ($\epsilon = 0.2$).

Figure 13: Relative error for CGLS, AB-GMRES and stabilized AB-GMRES for Maragal3T ($\epsilon = 0.5$).
Table 6: Information of the singular square matrices.

| matrix      | size | density[\%] | rank | \(\kappa_2(A)\) | application                      |
|-------------|------|-------------|------|------------------|---------------------------------|
| Harvard500  | 500  | 1.05        | 170  | 1.30 \times 10^2 | web connectivity                |
| netz4504    | 1961 | 0.13        | 1342 | 3.41 \times 10^3 | 2D/3D finite element problem    |
| TS          | 2142 | 0.99        | 2140 | 3.52 \times 10^3 | counter example problem         |
| grid2\_dual | 3136 | 0.12        | 3134 | 8.58 \times 10^3 | 2D/3D finite element problem    |
| uk          | 4828 | 0.06        | 4814 | 6.62 \times 10^3 | undirected graph                |
| bw42        | 10000| 0.05        | 9999 | 2.03 \times 10^3 | partial differential equation[4] |

Table 7: Comparison of the attainable smallest relative residual norm \(\|A^T r_i\|_2/\|A^T r_0\|_2\) for inconsistent square linear systems.

| matrix      | Harvard500 | netz4504 | TS    | grid2\_dual | uk  | bw42 |
|-------------|-------------|----------|-------|-------------|-----|------|
| iter.       | 104         | 144      | 1487  | 3134        | 4620| 715  |
| standard AB-GMRES | 9.38 \times 10^{-9} | 4.51 \times 10^{-10} | 1.56 \times 10^{-9} | 5.98 \times 10^{-10} | 1.35 \times 10^{-9} | 8.06 \times 10^{-8} |
| iter.       | 175         | 201      | 1617  | 3135        | 4779| 788  |
| stabilized AB-GMRES | 1.53 \times 10^{-14} | 1.51 \times 10^{-14} | 1.54 \times 10^{-9} | 1.14 \times 10^{-9} | 6.81 \times 10^{-10} | 1.66 \times 10^{-7} |
| iter.       | 135         | 200      | 1652  | 3134        | 4706| 1163 |
| RR-AB-GMRES | 7.78 \times 10^{-14} | 3.36 \times 10^{-14} | 4.56 \times 10^{-9} | 6.52 \times 10^{-8} | 8.33 \times 10^{-8} | 1.56 \times 10^{-5} |
| iter.       | 139         | 194      | 1628  | 3134        | 4724| 1520 |
| BA-GMRES    | 1.91 \times 10^{-15} | 7.27 \times 10^{-16} | 8.43 \times 10^{-13} | 1.23 \times 10^{-13} | 6.94 \times 10^{-14} | 1.97 \times 10^{-11} |
| iter.       | 391         | 198      | 6047  | 12549       | 6249| 1256 |
| LSQR        | 3.59 \times 10^{-15} | 5.86 \times 10^{-16} | 1.96 \times 10^{-12} | 2.51 \times 10^{-13} | 6.56 \times 10^{-14} | 1.59 \times 10^{-11} |
| iter.       | 338         | 195      | 6219  | 12497       | 6199| 1212 |
| LSMR        | 2.01 \times 10^{-15} | 5.97 \times 10^{-16} | 1.25 \times 10^{-12} | 2.34 \times 10^{-13} | 7.35 \times 10^{-14} | 1.60 \times 10^{-11} |

\(\epsilon = 0.2\) and \(\epsilon = 0.5\), whose \(|b|_{\mathcal{N}(A^T)}_2/\|b\|_{\mathcal{R}(A)}_2 \geq 0.05\).

5.3 Inconsistent systems with highly ill-conditioned square coefficient matrices

The stabilized AB-GMRES is not restricted to solving underdetermined problems but can also be applied to solving the least squares problem
\[
\min_{x \in \mathbb{R}^n} \|b - Ax\|_2,
\]
where \(A \in \mathbb{R}^{n \times n}\) is a highly ill-conditioned square matrix. Thus, we also test on square matrices of different kinds. Table 6 gives the information of the matrices.

These matrices are all numerically singular. We generated the right-hand side \(b\) by the MATLAB function \texttt{rand}, so that the systems are generically inconsistent. We compared the stabilized AB-GMRES with the standard AB-GMRES, RR-AB-GMRES, BA-GMRES with \(B = A^T\), LSMR [7], and LSQR [20]. Table 7 gives the smallest relative residual norm and the number of iterations. Table 7 gives the CPU times in seconds required to obtain relative residual norm \(\|A^T r_i\|_2/\|A^T r_0\|_2 < 10^{-8}\). The switching strategy which was introduced in Section 4.1 was used for the stabilized AB-GMRES when measuring CPU times. The number of iterations when switching occurred is in brackets.

Table 7 shows that for most problems the BA-GMRES was the best in terms of accuracy of relative residual norm. The LSQR and LSMR are similar and are comparable to the BA-GMRES, because they all change the inconsistent problem into a consistent problem. The LSQR and LSMR are more suitable for large and sparse problems compared to the BA-GMRES because they require less CPU time and memory.

For Harvard500 and bw42, the AB-GMRES could only converge to the level of \(10^{-9}\) regarding the relative residual norm, while the stabilized AB-GMRES converged to the level of \(10^{-14}\). The stabilized AB-GMRES
Table 8: Attainable smallest relative residual norm $\| A^T r_i \|_2 / \| A^T r_0 \|_2$ for bw42.

| method            | iter. | min $\| A^T r_i \|_2 / \| A^T r_0 \|_2$ |
|-------------------|-------|----------------------------------------|
| standard GMRES    | 147   | $8.08 \times 10^{-9}$                  |
| stabilized GMRES  | 219   | $1.94 \times 10^{-11}$                 |
| RR-GMRES          | 220   | $3.13 \times 10^{-11}$                 |

Table 9: Comparison of the CPU time (seconds) to obtain relative residual norm $\| A^T r_i \|_2 / \| A^T r_0 \|_2 < 10^{-8}$ for inconsistent square linear systems.

| matrix            | Harvard500 | netz4504 | TSgrid2_dual | uk         | bw42  |
|-------------------|-------------|----------|--------------|------------|-------|
| iter.             | 104         | 134      | 1411         | 3134       | 4583  |
| standard AB-GMRES |             |          |              |            |       |
| iter.             | 104         | 134      | 1411         | 3134       | 4583  |
| stabilizd AB-GMRES|             |          |              |            |       |
| RR-AB-GMRES       |             |          |              |            |       |
| iter.             | 114         | 153      | 1530         | -          |       |
| BA-GMRES          |             |          |              |            |       |
| iter.             | 222         | 134      | 4239         | 11802      | 5948  |
| LSQR              |             |          |              |            |       |
| iter.             | 215         | 132      | 3913         | 11746      | 5898  |
| LSMR              |             |          |              |            |       |
was robust in the sense that it could continue to compute even when the upper triangular matrix $R_t$ became seriously ill-conditioned, and the relative residual norm did not increase sharply towards the end, but just stagnated at a low level, just like for consistent problems. Comparing the CPU time in Table 6, LSMR was the fastest. The stabilized AB-GMRES was usually faster than BA-GMRES.

Thus, our stabilization method also makes AB-GMRES stable for highly ill-conditioned inconsistent systems with square coefficient matrices.

The coefficient matrix $A$ of bw42 is singular and satisfies $\mathcal{N}(A) = \mathcal{N}(A^T)$. The problem comes from a finite-difference discretization of a PDE with periodic boundary condition (Experiment 4.2 in Brown and Walker [2] with the original $b$). Since the matrix is range symmetric, the GMRES, RR-GMRES, and stabilized GMRES can be directly applied to $Ax = b$ (See [4] Theorem 2.4, [9] Theorem 2.7, and [5] Theorem 3.2) as shown in Table 6. The stabilized GMRES gave the relative residual norm $1.94 \times 10^{-11}$ for bw42 at the 219th iteration, similar to the BA-GMRES.

6 Concluding Remarks

We proposed a stabilized AB-GMRES method for ill-conditioned underdetermined and inconsistent least squares problems. It shifts upwards the tiny singular values of the upper triangular matrix appearing in AB-GMRES, making the process more stable, giving better convergence, and more accurate solutions compared to AB-GMRES. The method is also effective for making AB-GMRES stable for inconsistent least squares problems with highly ill-conditioned square coefficient matrices.

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A Proof of statement in section 2.3

**Lemma 9.** Assume $\mathcal{N}(\tilde{A}) \cap \mathcal{R}(\tilde{A}) = \{0\}$, and $\text{grade}(\tilde{A}, b|_{R(\tilde{A})}) = k$. Then, $K_{k+1}(\tilde{A}, b|_{R(\tilde{A})}) = \tilde{A}K_k(\tilde{A}, b|_{R(\tilde{A})})$ holds.

**Proof.** Note that

$$\tilde{A}K_k(\tilde{A}, b|_{R(\tilde{A})}) = \text{span}\{\tilde{A}b|_{R(\tilde{A})}, \tilde{A}^2b|_{R(\tilde{A})}, \ldots, \tilde{A}^kB|_{R(\tilde{A})}\} \subseteq \text{span}\{b|_{R(\tilde{A})}, \tilde{A}b|_{R(\tilde{A})}, \ldots, \tilde{A}^kb|_{R(\tilde{A})}\} = K_{k+1}(\tilde{A}, b|_{R(\tilde{A})}).$$

grade($\tilde{A}, b|_{R(\tilde{A})}$) = $k$ implies that

$$K_{k+1}(\tilde{A}, b|_{R(\tilde{A})}) = \tilde{A}K_k(\tilde{A}, b|_{R(\tilde{A})}) = \text{span}\{b|_{R(\tilde{A})}, \tilde{A}b|_{R(\tilde{A})}, \ldots, \tilde{A}^{k-1}b|_{R(\tilde{A})}\}.$$

Hence,

$$\tilde{A}^kb|_{R(\tilde{A})} = c_0b|_{R(\tilde{A})} + c_1\tilde{A}b|_{R(\tilde{A})} + \cdots + c_{k-1}\tilde{A}^{k-1}b|_{R(\tilde{A})}, \quad c_i \in \mathbb{R}, i = 0, 1, 2, \ldots, k - 1.$$

If $c_0 = 0$,

$$\tilde{A}^kb|_{R(\tilde{A})} = c_1\tilde{A}b|_{R(\tilde{A})} + c_2\tilde{A}^2b|_{R(\tilde{A})} + \cdots + c_{k-1}\tilde{A}^{k-1}b|_{R(\tilde{A})}.$$

Hence,

$$c_1\tilde{A}b|_{R(\tilde{A})} + c_2\tilde{A}^2b|_{R(\tilde{A})} + \cdots + c_{k-1}\tilde{A}^{k-1}b|_{R(\tilde{A})} - \tilde{A}^kb|_{R(\tilde{A})} = \tilde{A}(c_1b|_{R(\tilde{A})} + \cdots + c_{k-1}\tilde{A}^{k-2}b|_{R(\tilde{A})} - \tilde{A}^{k-1}b|_{R(\tilde{A})}) = 0.$$
Hence,
\[ c_1b|_{\mathcal{R}(\tilde{A})} + c_2\tilde{A}^2b|_{\mathcal{R}(\tilde{A})} + \cdots + c_{k-1}\tilde{A}^{k-2}b|_{\mathcal{R}(\tilde{A})} - \tilde{A}^{k-1}b|_{\mathcal{R}(\tilde{A})} \in \mathcal{N}(\tilde{A}) \cap \mathcal{R}(\tilde{A}) = \{0\} \]
which implies
\[ \tilde{A}^{k-1}b|_{\mathcal{R}(\tilde{A})} = c_1b|_{\mathcal{R}(\tilde{A})} + c_2\tilde{A}b|_{\mathcal{R}(\tilde{A})} + \cdots + c_{k-1}\tilde{A}^{k-2}b|_{\mathcal{R}(\tilde{A})}. \]
Thus,
\[ \mathcal{K}_k(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = \mathcal{K}_{k-1}(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}), \]
which contradicts with grade\((\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = k\). Hence, \(c_0 \neq 0\), and
\[ b|_{\mathcal{R}(\tilde{A})} = d_1\tilde{A}b|_{\mathcal{R}(\tilde{A})} + d_2\tilde{A}^2b|_{\mathcal{R}(\tilde{A})} + \cdots + d_{k-1}\tilde{A}^{k-1}b|_{\mathcal{R}(\tilde{A})} + d_k\tilde{A}^kb|_{\mathcal{R}(\tilde{A})}. \]
Hence,
\[ \mathcal{K}_{k+1}(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = \text{span}\{b|_{\mathcal{R}(\tilde{A})}, \tilde{A}b|_{\mathcal{R}(\tilde{A})}, \cdots, \tilde{A}^kb|_{\mathcal{R}(\tilde{A})}\} \subseteq \text{span}\{\tilde{A}b|_{\mathcal{R}(\tilde{A})}, \tilde{A}^2b|_{\mathcal{R}(\tilde{A})}, \cdots, \tilde{A}^kb|_{\mathcal{R}(\tilde{A})}\} = \tilde{A}\mathcal{K}_k(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}). \]
Thus,
\[ \mathcal{K}_{k+1}(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = \tilde{A}\mathcal{K}_k(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}). \]

Corollary 10. Assume \(\mathcal{N}(\tilde{A}) = \mathcal{N}(\tilde{A}^T)\), and grade\((\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = k\). Then, \(\mathcal{K}_{k+1}(\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = \tilde{A}\mathcal{K}_k(\tilde{A}, b|_{\mathcal{R}(\tilde{A})})\) holds.

Proof. \(\mathcal{N}(\tilde{A}) = \mathcal{N}(\tilde{A}^T)\) implies that
\[ \mathcal{N}(\tilde{A}) \cap \mathcal{R}(\tilde{A}) = \mathcal{N}(\tilde{A}^T) \cap \mathcal{R}(\tilde{A}) = \mathcal{R}(\tilde{A})^\perp \cap \mathcal{R}(\tilde{A}) = \{0\}. \]
Hence, from Lemma 9, Corollary 10 holds.

B Proof of statement in section 2.3

Lemma 11. Assume \(\mathcal{N}(\tilde{A}) \cap \mathcal{R}(\tilde{A}) = \{0\}\), grade\((\tilde{A}, b|_{\mathcal{R}(\tilde{A})}) = k\), and \(b \notin \mathcal{R}(\tilde{A})\). Then, \(\text{dim}(K_{k+1}(\tilde{A}, b)) = k + 1\) holds.

Proof. Let \(c_0, c_1, \ldots, c_k \in \mathbb{R}\) satisfy
\[ c_0b + c_1\tilde{A}b + \cdots + c_k\tilde{A}^kb = 0. \]
Since \(\mathcal{N}(\tilde{A}) \cap \mathcal{R}(\tilde{A}) = \{0\}\),
\[ b = b|_{\mathcal{R}(\tilde{A})} \oplus b|_{\mathcal{N}(\tilde{A})}, \]
where \(b|_{\mathcal{N}(\tilde{A})}\) denotes the orthogonal projection of \(b\) onto \(\mathcal{N}(\tilde{A})\). Hence,
\[ c_0b|_{\mathcal{N}(\tilde{A})} + c_0b|_{\mathcal{R}(\tilde{A})} + c_1\tilde{A}b|_{\mathcal{R}(\tilde{A})} + \cdots + c_k\tilde{A}^kb|_{\mathcal{R}(\tilde{A})} = 0. \]
If \(c_0 \neq 0\)
\[ b|_{\mathcal{N}(\tilde{A})} = -\frac{c_1}{c_0}\tilde{A}b|_{\mathcal{R}(\tilde{A})} - \cdots - \frac{c_k}{c_0}\tilde{A}^kb|_{\mathcal{R}(\tilde{A})} \in \mathcal{R}(\tilde{A}). \]
Hence,
\[ b|_{\mathcal{N}(\tilde{A})} \in \mathcal{N}(\tilde{A}) \cap \mathcal{R}(\tilde{A}) = \{0\}. \]
Thus, \( b|_{N(A)} = 0 \), which contradicts \( b \notin R(A) \). Hence, we have \( c_0 = 0 \), and

\[
c_1 \tilde{A}b + c_2 \tilde{A}^2 b + \cdots + c_k \tilde{A}^k b = c_1 A b|_{R(A)} + c_2 \tilde{A}^2 b|_{R(A)} + \cdots + c_k \tilde{A}^k b|_{R(A)} = 0.
\]

But, since

\[
\dim(\text{span}\{\tilde{A}b|_{R(A)}, \tilde{A}^2 b|_{R(A)}, \cdots, \tilde{A}^k b|_{R(A)}\}) = \dim(\text{span}\{b|_{R(A)}, \tilde{A}b|_{R(A)}, \cdots, \tilde{A}^k b|_{R(A)}\}) = \dim(A K_k(\tilde{A}, b|_{R(A)})) = k
\]
holds from Lemma 9 we have \( c_1 = c_2 = \cdots = c_k = 0 \), which implies \( \dim(K_{k+1}(\tilde{A}, b)) = k + 1 \).

\[\square\]

**Corollary 12.** Assume \( N(A) = N(\tilde{A}^T) \), \( \text{grade}(\tilde{A}, b|_{R(\tilde{A})}) = k \), and \( b \notin R(\tilde{A}) \).

Then, \( \dim(K_{k+1}(\tilde{A}, b)) = k + 1 \) holds.

**Proof.** \( N(\tilde{A}) = N(\tilde{A}^T) \) implies \( N(\tilde{A}) \cap R(\tilde{A}) = \{0\} \). Hence, the corollary follows from Lemma 11.

\[\square\]

### C Proof of Theorem 7 in section 4.4

**Theorem 7** Let \( R_s = (r_{pq}) \in \mathbb{R}^{s \times s} \) be an upper-triangular matrix and

\[
R_{s+1} = \begin{pmatrix} R_s & d \\ 0^T & r_{s+1, s+1} \end{pmatrix} \in \mathbb{R}^{(s+1) \times (s+1)}.
\]  

Assume \( R_s \) is numerically nonsingular, and \( R_s = O(1), R_s^{-1} = O(1), M(R_s)^{-1} = O(1), d = O(1) \) and \( O(s) = O(s^2) = O(1) \). Then, the following holds:

\[
\operatorname{fl}(R_{s+1}^T R_{s+1}) \text{ is numerically nonsingular } \iff \operatorname{fl}(r_{s+1, s+1}^2) > \operatorname{fl}(d^T d) O(\epsilon).
\]

**Proof.** Note that

\[
R_{s+1}^T R_{s+1} = \begin{pmatrix} R_s & 0 \\ d^T & r_{s+1, s+1} \end{pmatrix} \begin{pmatrix} R_s & d \\ 0^T & r_{s+1, s+1} \end{pmatrix} = \begin{pmatrix} R_s^T R_s & R_s^T d \\ d^T R_s & d^T d + r_{s+1, s+1}^2 \end{pmatrix}.
\]

Proof of \((\Rightarrow)\)

Assume \( \operatorname{fl}(r_{s+1, s+1}^2) \leq \operatorname{fl}(d^T d) O(\epsilon) \). Then, since

\[
\operatorname{fl}(d^T d) = d^T d + O(\epsilon) d^T d = (1 + O(\epsilon)) d^T d,
\]

\[
\operatorname{fl}(d^T d + r_{s+1, s+1}^2) = (d^T d + r_{s+1, s+1}^2)(1 + O(\epsilon)) = d^T d(1 + O(\epsilon)),
\]

we have

\[
\operatorname{fl}(R_{s+1}^T R_{s+1}) = \begin{pmatrix} R_s^T R_s + O(\epsilon)|R_s||R_s| & R_s^T d + O(\epsilon)|R_s||R_s| \\ d^T R_s + O(\epsilon)|d||R_s| & d^T d + O(\epsilon)d^T d \end{pmatrix} = \begin{pmatrix} R_s^T R_s & R_s^T d \\ d^T R_s & d^T d + O(\epsilon)d^T d \end{pmatrix} + O(\epsilon),
\]

since \( R_s = O(1) \) and \( d = O(1) \). Note

\[
\begin{pmatrix} R_s & d \\ 0^T & 1 \end{pmatrix} \begin{pmatrix} -R_s^{-1} d \\ 1 \end{pmatrix} = -R_s R_s^{-1} d + d = 0,
\]

since \( R_s \) is nonsingular.
Hence,
\[
\mathfrak{f}(R_s d \begin{pmatrix} -R_s^{-1}d \\ 1 \end{pmatrix}) = \mathfrak{f}(R_s \mathfrak{f}(-R_s^{-1}d) + d) = |\mathfrak{f}(R_s \mathfrak{f}(-R_s^{-1}d)) + d| (1 + O(\varepsilon)).
\]

Note here that
\[
\mathfrak{f}(R_s \mathfrak{f}(-R_s^{-1}d)) = R_s \mathfrak{f}(-R_s^{-1}d) + O(\varepsilon) |R_s||R_s^{-1}d|,
\]
and
\[
\mathfrak{f}(-R_s^{-1}d) = -R_s^{-1}d + O(s^2 \varepsilon) M(R_s)^{-1} |d|
\]
from Theorem 6. Hence,
\[
O((s^2 \varepsilon) R_s M(R_s)^{-1} |d| + O(\varepsilon) |R_s||R_s^{-1}d| = \Theta(s^2 \varepsilon),
\]
since \( R_s^{-1} = O(1) \) and \( M(R_s)^{-1} = O(1) \).

Then,
\[
\mathfrak{f}(R_{s+1}^T R_{s+1} \begin{pmatrix} -R_s^{-1}d \\ 1 \end{pmatrix}) = \mathfrak{f}(\left\{ \begin{pmatrix} R_s^T \\ 1 \end{pmatrix} \begin{pmatrix} d \\ R_s \end{pmatrix} + O(\varepsilon) \left\{ \begin{pmatrix} -R_s^{-1}d \\ 1 \end{pmatrix} \right\} \right\} (R_s R_{s+1} + O((s + 1) \varepsilon)) + |R_{s+1}^T R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix} + |R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix} + O((s + 1) \varepsilon)) = \Theta(s) = \Theta(\varepsilon),
\]
since 34, 35, and \( O(s^2) = O(1) \). Since \( \left\{ \begin{pmatrix} -R_s^{-1}d \\ 1 \end{pmatrix} \right\} = \Theta(1) \), \( R_{s+1}^T R_{s+1} \) is numerically singular. By contraposition, \( \Rightarrow \) holds.

Proof of \( \Leftarrow \)

Assume \( R_{s+1}^T R_{s+1} \) is not numerically singular. Then, there exists a vector \( \begin{pmatrix} z \\ w \end{pmatrix} \in \mathbb{R}^{s+1} \) such that
\[
\left| \begin{pmatrix} z \\ w \end{pmatrix} \right| > \Theta(\varepsilon),
\]
and
\[
\mathfrak{f}(R_{s+1}^T R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix}) = R_{s+1}^T \begin{pmatrix} R_s \begin{pmatrix} z \\ w \end{pmatrix} + |R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix} + O((s + 1) \varepsilon)) + |R_{s+1}^T R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix} + |R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix} + O((s + 1) \varepsilon)) = \Theta(\varepsilon)
\]
assuming \( O(s + 1) = O(1) \).

Hence,
\[
\mathfrak{f}(R_{s+1}^T R_{s+1} \begin{pmatrix} z \\ w \end{pmatrix}) = \left( \begin{pmatrix} R_s^T d \\ d^T R_s \end{pmatrix} + R_{s+1}^T \begin{pmatrix} z \\ w \end{pmatrix} \right) + \Theta(\varepsilon) = \Theta(\varepsilon)
\]
Thus,
\[
R_s^T R_s z + w R_s^T d = \Theta(\varepsilon),
\]
\[
d^T R_s z + (d^T d + r_{s+1, s+1}^2) w = \Theta(\varepsilon).
\]
(36) can be expressed as \( R_s^T (R_s z + w d) = \Theta(\varepsilon) \). From Lemma 13, \( R_s^T \) is numerically nonsingular, so that
\[
R_s z + wd = \Theta(\varepsilon).
\]
Hence, from (37), \( d^T R_s z + w(d^T d + r_{s+1, s+1}^2) = d^T (R_s z + w d) + wr_{s+1, s+1}^2 = \Theta(\varepsilon) \). Thus, \( wr_{s+1, s+1}^2 = \Theta(\varepsilon) \).

If \( w = \Theta(\varepsilon) \), \( R_s z = \Theta(\varepsilon) \) from 35. Since \( R_s \) is numerically nonsingular, \( z = \Theta(\varepsilon) \), which contradicts with the assumption.
Hence, \(|w| > O(\epsilon)\), so that \(r_{s+1,s+1}^2 = O(\epsilon)\), which gives
\[
\mathfrak{f}(r_{s+1,s+1}^2) = O(\epsilon) \leq \mathfrak{f}(d^T d)O(\epsilon).
\]

\[\square\]

**Lemma 13.** Let \(n = O(1)\). If \(A \in \mathbb{R}^{n \times n}\) is numerically nonsingular, and \(A^{-1} = O(1)\), then \(A^T\) is numerically nonsingular.

**Proof.** If
\[
\mathfrak{f}(A^T x) = A^T x + O(ne)||A^T||x| = O(ne),
\]
then
\[
\mathfrak{f}(x^T A) = x^T A + O^T(n) = O^T(n).
\]
Thus,
\[
\mathfrak{f}(x^T Ay) = \mathfrak{f}(x^T A)y + O(ne)||x^T A||y| = O(ne)
\]
holds for all \(y = O(1)\).

For arbitrary \(z = O(1) \in \mathbb{R}^n\), let
\[
y = A^{-1} z = O(1).
\]
Then,
\[
\mathfrak{f}(Ay) = Ay + O(ne)||A||y| = z + O(ne)||A||y|.
\]
Hence,
\[
z = \mathfrak{f}(Ay) + O(ne)||A||y| = \mathfrak{f}(Ay) + O(ne).
\]
Thus, we have
\[
\mathfrak{f}(x^T z) = x^T z + O(ne)||x^T z| = \mathfrak{f}(x^T Ay) + O(ne) = O(ne)
\]
for arbitrary \(z = O(1) \in \mathbb{R}^n\). Hence, \(x = O(\epsilon)\), so that \(A^T\) is numerically nonsingular. \[\square\]

**D  Proof of Theorem \(\S\) in section 4.5**

**Proof.** Let the singular value decomposition of \(R_i\) be given by \(R_i = U \Sigma V^T \in \mathbb{R}^{i \times i}\), where \(U, V\) are orthogonal matrices and \(\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_i)\). Let \(I_i \in \mathbb{R}^{i \times i}\) be the identity matrix. Then, we have
\[
R_i' = \left( \begin{array}{c} R_i \\ \sqrt{\lambda_i} \end{array} \right) = U' \Sigma' V^T, \text{ where } U' = \left( \begin{array}{cc} U & 0 \\ 0 & V \end{array} \right) \text{ and } \Sigma' = \left( \begin{array}{c} \Sigma \\ \sqrt{\lambda_i} \end{array} \right). \text{ Since } \Sigma'^T \Sigma' = \Sigma^2 + \lambda_i = \text{diag}(\sigma_1^2 + \lambda, \sigma_2^2 + \lambda, \ldots, \sigma_i^2 + \lambda), \text{ the singular values of } \left( \begin{array}{c} R_i \\ \sqrt{\lambda_i} \end{array} \right) \text{ are } \sqrt{\sigma_1^2 + \lambda} \geq \sqrt{\sigma_2^2 + \lambda} \geq \cdots \geq \sqrt{\sigma_i^2 + \lambda}. \[\square\]

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