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GMRES-type methods for inconsistent systems

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To Robert J. Plemmons for his singular dedication to Linear Algebra

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Abstract

The behavior of iterative methods of GMRES-type when applied to singular, possibly inconsistent, linear systems is discussed and conditions under which these methods converge to the least-squares solution of minimal norm are presented. Error bounds for the computed iterates are shown. This paper complements previous work by Brown and Walker [P.N. Brown, H.F. Walker, SIAM J. Matrix Anal. Appl. 18 (1997) 37–51]. © 2000 Elsevier Science Inc. All rights reserved.

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1. Introduction

The GMRES method by Saad and Schulz [6] is one of the most popular iterative methods for the solution of large linear systems of equations

$$Ax = b, \quad A \in \mathbb{R}^{n\times n},\ x, b \in \mathbb{R}^n \tag{1.1}$$

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with a nonsymmetric and nonsingular matrix A. Let x_0 be a given initial approximate solution of (1.1) and let $r_0 = b - Ax_0$ be the associated residual vector. Introduce the Krylov spaces

$$\mathcal{K}_m(A, r_0) = \text{span}\left\{r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0\right\}, \quad m = 1, 2, \ldots$$

The GMRES method determines for an arbitrary value of $m \geqslant 1$ a correction $d_m \in \mathcal{K}_m(A, r_0)$ of x_0, such that the improved approximate solution $x_m = x_0 + d_m$ satisfies

$$\|Ax_m - b\| = \min_{d_m \in \mathcal{K}_m(A, r_0)} \|A(x_0 + d_m) - b\|. \tag{1.2}$$

Here and below $\|\cdot\|$ denotes the Euclidean vector norm or the associated induced operator norm.

It is easy to see, e.g., by using the Jordan normal form of A, that there is an integer ℓ, such that

$$\dim \mathcal{K}_m(A, r_0) = \begin{cases} m, & m \leqslant \ell, \\ \ell, & m \geqslant \ell. \end{cases} \tag{1.3}$$

Throughout this paper, the integer ℓ is defined by (1.3). Saad and Schulz [6, Proposition 2] show that, when A is nonsingular and $m \geqslant \ell$, the solution x_m of the minimization problem (1.2) solves the linear system (1.1).

The GMRES method is often implemented by first computing an orthogonal basis $\{v_j\}_{j=1}^{\min\{m,\ell\}}$ of the Krylov subspace $\mathcal{K}_m(A, r_0)$ by Arnoldi's method; see [6] or [7]. Let $k = \min\{m, \ell\}$. Arnoldi's method yields the decomposition

$$AV_k = V_k H_k + f_k e_k^{\mathrm{T}}, \tag{1.4}$$

where $H_k = [h_{i,j}]_{i,j=1}^{k} \in \mathbb{R}^{k\times k}$ is an upper Hessenberg matrix, $V_k = [v_1, v_2, \ldots, v_k] \in \mathbb{R}^{n\times k}$, $V_k^{\mathrm{T}} V_k = I_k$, $V_k e_1 = r_0/\|r_0\|$ and $V_k^{\mathrm{T}} f_k = 0$. Throughout this paper I_k denotes the identity matrix of order k and e_j denotes the jth axis vector. It follows from (1.3) that $f_k \neq 0$ for $0 \leqslant k < \ell$ and $f_\ell = 0$.

When $f_k \neq 0$, the decomposition (1.4) can also be written in the form

$$AV_k = V_{k+1}\bar{H}_k, \tag{1.5}$$

where $V_{k+1} \in \mathbb{R}^{n\times(k+1)}$ is obtained by appending the vector $v_{k+1} = f_k/\|f_k\|$ to V_k and $\bar{H}_k \in \mathbb{R}^{(k+1)\times k}$ is obtained by appending the row $\|f_k\| e_k^{\mathrm{T}}$ to H_k. Note that $V_{k+1}^{\mathrm{T}} V_{k+1} = I_{k+1}$ and that $\bar{H}_k$ is of Hessenberg-type. We state Arnoldi's method for the sake of completeness.

Algorithm 1.1 (*Arnoldi's method*).

Input: *matrix A, initial vector* r_0, *maximum number of steps m*;

Output: $k := \min\{m, \ell\}$, $H_k = [h_{i,j}]$, $V_k = [v_1, v_2, \ldots, v_k]$, f_k *in the Arnoldi decomposition* (1.4);

$f_0 := r_0$;

for $j = 1, 2, \ldots, m$ *do*

if $\|f_{j-1}\| = 0$ *then* $k := j$; *exit endif*;
$v_j := f_{j-1}/\|f_{j-1}\|$;
if $j > 0$ *then* $h_{j,j-1} := \|f_{j-1}\|$ *endif*;
$f_j := Av_j$;
for $i = 1, 2, \ldots, j$ *do*

$$h_{i,j} := v_i^{\mathrm{T}} f_j;\ f_j := f_j - h_{i,j} v_i;$$

endfor i;

endfor j;
$k := m$;

Arnoldi's method *breaks down* at step $\ell + 1$, because $f_\ell = 0$ and the computations with the algorithm cannot be continued. We note that when Arnoldi's method breaks down at step $\ell + 1$, an orthogonal Krylov space basis of dimension ℓ has been determined.

Using the Arnoldi decomposition (1.5) and the fact that $d_m = V_k y_k$ for some $y_k \in \mathbb{R}^k$, the minimization problem (1.2) can be written in the form

$$\begin{aligned}\min_{d_m \in \mathcal{K}_m(A,r_0)} \|A(x_0 + d_m) - b\| &= \min_{y_k \in \mathbb{R}^k} \|AV_k y_k - r_0\| \\ &= \min_{y_k \in \mathbb{R}^k} \left\| V_{k+1} \left(\bar{H}_k y_k - \|r_0\| e_1 \right) \right\| \\ &= \min_{y_k \in \mathbb{R}^k} \left\| \bar{H}_k y_k - \|r_0\| e_1 \right\|. \end{aligned} \tag{1.6}$$

When $f_k = 0$, the matrix $\bar{H}_k$ in (1.6) should be replaced by H_k. This occurs for $m \geqslant \ell$, where ℓ is defined by (1.3).

Analogously with the terminology used for Arnoldi's method, we say that the GMRES method breaks down at step $\ell + 1$. A difficulty that arises when applying the GMRES method to linear systems with a singular matrix is that the method may break down before the generated Krylov space is large enough to contain the desired correction of x_0.

Example 1.1. Let

$$A = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad b = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad x_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{1.7}$$

Then $r_0 = (0, 1)^{\mathrm{T}}$ and $Ar_0 = (0, 0)^{\mathrm{T}}$. Thus, $\ell = 1$ in (1.3) and Arnoldi's method breaks down with $k = 1$. We, therefore, are not able to improve the initial approximate solution x_0. We remark that any vector $x = [1, \xi]^{\mathrm{T}}$, $\xi \in \mathbb{R}$, solves the linear system (1.1).

The present paper studies the behavior of the GMRES method when the matrix A is singular. We are particularly interested in the performance of the GMRES method when the linear system (1.1) is inconsistent. Our investigation complements the recent study by Brown and Walker [3], and we apply several of the results and the techniques developed in [3].

A nice survey of properties of the GMRES method when applied to consistent linear systems with a singular matrix A is provided by Ipsen and Meyer [4]. Let $\mathscr{R}(A)$ and $\mathscr{N}(A)$ denote the range and null space of the matrix A, respectively. Assume that A is singular, and let the zero eigenvalue have index i, i.e., the largest Jordan block associated with the zero eigenvalue is of order i. Let $x_0 = 0$. Ipsen and Meyer [4] show that the GMRES method then produces a solution of the linear system (1.1) if and only if $b \in \mathscr{R}(A^i)$. We are therefore led to study under which conditions the GMRES method yields a least-squares solution of (1.1) for a general right-hand side vector b.

According to (1.2) the GMRES method produces a solution to a constrained least-squares problem; the minimization is constrained to the Krylov space $\mathscr{K}_m(A, r_0)$. We would like to investigate under which conditions on A and b, the solution x_m of the constrained least-squares problem (1.2) is a least-squares solution of the system (1.1), i.e., when

$$\min_{d_m \in \mathscr{K}_m(A,r_0)} \|b - A(x_0 + d_m)\| = \min_{x \in \mathbb{R}^n} \|b - Ax\| \tag{1.8}$$

or, equivalently, when the solution $x_m = x_0 + d_m$ of (1.2) satisfies the normal equations

$$A^{\mathrm{T}}Ax = A^{\mathrm{T}}b. \tag{1.9}$$

The minimization problem (1.8), or, equivalently, the normal equations (1.9), do not have a unique solution when A is singular. We are interested in when the GMRES method determines the solution of minimal norm. For future reference, we denote this solution by $x^{\dagger}$. It is characterized by being the unique solution of (1.9) in $\mathscr{N}(A)^{\perp}$; this can be seen by substituting the singular value decomposition of A into (1.9).

The close connection between the minimization problem (1.2) and the normal equations (1.9) helps us to shed some light on the question whether it is possible to compute a least-squares solution to overdetermined systems of equations by an iterative method without using the transpose of the matrix.[3]

This paper is organized as follows. In the remainder of this section, we introduce notation to be used throughout the paper. Section 2 discusses the behavior of the GMRES method for the solution of consistent and inconsistent singular linear systems. In Section 3, we present a modification of the GMRES method, referred to as RRGMRES, that restricts the computed solution to $\mathscr{R}(A)$, and we show why this modification can be beneficial. Bounds for the distance between the approximate

[3] This question was raised by Bob Plemmons at a conference in DeKalb a few years ago.

solutions computed by the GMRES or RRGMRES methods and the minimal norm least-squares solution of (1.1) are discussed in Section 4. Throughout Sections 2–4, we assume that A is an n by n matrix. Section 5 applies the results of the previous sections to the case when A is an m by n matrix, with $m > n$, and Section 6 contains concluding remarks.

We conclude this section by introducing notation and definitions to be used in the sequel. A matrix A is said to be *range symmetric* if $\mathcal{R}(A) = \mathcal{R}(A^{\mathrm{T}})$. Range symmetric matrices include symmetric matrices and skew-symmetric matrices.

We may assume that $x_0 = 0$ and then the associated residual vector is $r_0 = b$. Throughout this paper we use the notation

$$\mathcal{K}_m = \mathcal{K}_m(A, b), \qquad \mathcal{K}_m^* = \mathcal{K}_m(A, Ab). \tag{1.10}$$

2. The GMRES method for singular systems

It follows from (1.3) that the GMRES method breaks down for the smallest value of m such that $\dim \mathcal{K}_m = \dim \mathcal{K}_{m+1} = m$. If the system is inconsistent, then breakdown will occur for the smallest value of m such that $\dim A\mathcal{K}_m = m - 1$. The following lemma is the central idea for relating the breakdown of GMRES to the least-squares problem (1.2). It was shown for the case when $\dim A\mathcal{K}_m = m$ by Brown and Walker [3, Proof of Lemma 2.3].

Lemma 2.1. *For all* $m \leqslant n$, $\dim A^{\mathrm{T}}A\mathcal{K}_m = \dim A\mathcal{K}_m$.

Proof. Clearly, $\dim A^{\mathrm{T}}A\mathcal{K}_m \leqslant \dim A\mathcal{K}_m$. Assume that $\dim A^{\mathrm{T}}A\mathcal{K}_m < \dim A\mathcal{K}_m$. We will see that this leads to a contradiction. Let $p = \dim A^{\mathrm{T}}A\mathcal{K}_m$. Then $\dim A\mathcal{K}_m \geqslant p + 1$ and, in particular, $m \geqslant p + 1$. Now, $\dim A^{\mathrm{T}}A\mathcal{K}_m = p$ if and only if there are coefficients $\alpha_1, \alpha_2, \ldots, \alpha_{p+1}$, not all zero, such that

$$\alpha_1 A^{\mathrm{T}}Ab + \alpha_2 A^{\mathrm{T}}A^2b + \cdots + \alpha_{p+1}A^{\mathrm{T}}A^{p+1}b = 0. \tag{2.1}$$

Let $z = \alpha_1 b + \alpha_2 Ab + \cdots + \alpha_{p+1}A^p b$. It follows from (2.1) that $A^{\mathrm{T}}Az = 0$. However, $\dim A\mathcal{K}_m \geqslant p + 1$ and therefore $Az = 0$ would imply that $\alpha_j = 0$ for $1 \leqslant j \leqslant p + 1$. Thus, $Az \neq 0$. This is a contradiction since, $0 < \|Az\|^2 = z^{\mathrm{T}}A^{\mathrm{T}}Az = 0$. Therefore, $\dim A^{\mathrm{T}}A\mathcal{K}_m = \dim A\mathcal{K}_m$. □

Theorem 2.2. *Apply the GMRES method to the linear system* (1.1) *until breakdown at step m. If* $\operatorname{rank}(A) = m - 1$, *then the GMRES method produces a least-squares solution of* (1.1).

Proof. We remark that the linear system (1.1) is not required to be consistent. Let $\operatorname{rank}(A) = m - 1$ and suppose that the GMRES method does not determine a least-squares solution of (1.1) at breakdown. Then there is no $x \in \mathcal{K}_m$ that satisfies the normal equations (1.9). In other words, $A^{\mathrm{T}}b \notin A^{\mathrm{T}}A\mathcal{K}_m$. By Lemma 2.1,

we have dim $A^{\mathrm{T}}A\mathscr{K}_m = \dim A\mathscr{K}_m = m-1$, and therefore dim $A^{\mathrm{T}}\mathscr{K}_m = m = \mathrm{rank}(A)+1$. However, $\mathrm{rank}(A) = \mathrm{rank}(A^{\mathrm{T}})$ and therefore dim $A^{\mathrm{T}}\mathscr{K}_m < m$, a contradiction. Thus, if $\mathrm{rank}(A) = m-1$ and the GMRES method breaks down at step m, then the method determines a least-squares solution. Indeed, since $A^{\mathrm{T}}A\mathscr{K}_{m-1} \subseteq A^{\mathrm{T}}A\mathscr{K}_m$ and dim $A^{\mathrm{T}}A\mathscr{K}_{m-1} = \dim A\mathscr{K}_{m-1} = m-1 = \dim A^{\mathrm{T}}A\mathscr{K}_m$, we have $A^{\mathrm{T}}A\mathscr{K}_{m-1} = A^{\mathrm{T}}A\mathscr{K}_m$. Therefore, the GMRES method determines a least-squares solution at step $m-1$ already. □

Example 2.1. Let

$$A = \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix}, \qquad b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad x_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{2.2}$$

The rank-one matrix A is not range symmetric. The GMRES method breaks down at step 2 producing the minimal norm least-squares solution $x_2 = (1/10, 2/10)^{\mathrm{T}}$.

Brown and Walker [3, Theorem 2.4] show that the GMRES method applied to the linear system (1.1) yields a least-squares solution for any right-hand side vector b if and only if the matrix is range symmetric. Theorem 2.2 and Example 2.1 complement this result by showing that a least-squares solution can be computed for linear systems with matrices that are not range symmetric.

The practical implication of these results is that if the matrix A is not range symmetric and if $\ell < \mathrm{rank}(A)$, where ℓ is defined by (1.3), then the GMRES method might not determine a least-squares solution of (1.1).

3. The range restricted GMRES method for singular systems

We introduce a variant of the GMRES method that has several advantages over the standard GMRES method discussed in Sections 1–2 when applied to the solution of linear systems of equations with a singular or nearly singular matrix. Our variant of the GMRES method is obtained by replacing the space $\mathscr{K}_m$ by $\mathscr{K}_m^*$ in the standard GMRES method; see (1.10) for a definition of these spaces. Thus, given the initial approximate solution $x_0 = 0$, the method determines an improved approximate solution x_m, such that

$$\|Ax_m - b\| = \min_{x \in \mathscr{K}_m^*} \|Ax - b\|. \tag{3.1}$$

Since all Krylov spaces $\mathscr{K}_m^*$, $m \geqslant 1$, are in $\mathscr{R}(A)$, we refer to this variant of the GMRES method as the *range restricted* GMRES method or briefly as the RRGMRES method.

The decomposition

$$\mathbb{R}^n = \mathscr{R}(A^{\mathrm{T}}) \oplus \mathscr{N}(A) \tag{3.2}$$

is useful for the investigation of the properties of the RRGMRES method. It is used in the proof of the following lemma, which shows that if $\mathcal{R}(A) = \mathcal{R}(A^{\mathrm{T}})$, then the RRGMRES method does not break down due to rank deficiency of $A\mathcal{K}_m^*$.

Lemma 3.1. *Suppose that* $\dim \mathcal{K}_m^* = m$ *and* $\mathcal{R}(A) = \mathcal{R}(A^{\mathrm{T}})$. *Then* $\dim A\mathcal{K}_m^* = m$.

Proof. Assume that $\dim A\mathcal{K}_m^* < m$. Then there is a $w \in \mathcal{K}_m^*$, $w \neq 0$, such that $Aw = 0$, i.e., w is a nontrivial element of $\mathcal{N}(A)$. However, $w \in \mathcal{K}_m^*$, and therefore $w \in \mathcal{R}(A)$. Hence, $w \in \mathcal{R}(A^{\mathrm{T}})$. It now follows from the decomposition (3.2) that $w = 0$. This contradiction shows that $\dim A\mathcal{K}_m^* = m$. □

By definition, $\dim \mathcal{K}_{m+1} = \ell = m = \dim \mathcal{K}_m$ at breakdown. This fact, together with Lemma 3.1, is the basis for the following result.

Theorem 3.2. *Assume that* $\mathcal{R}(A) = \mathcal{R}(A^{\mathrm{T}})$. *Then the RRGMRES method applied to the linear system* (1.1) *produces the minimal norm least-squares solution.*

Proof. We remark that the result holds for any right-hand side vector $b \in \mathbb{R}^n$ in (1.1). Suppose that the RRGMRES method breaks down at step $m+1$, i.e., $\dim \mathcal{K}_{m+1}^* = m$. In order for the RRGMRES method to be able to determine a least-squares solution, it is necessary and sufficient that there is an element $w \in \mathcal{K}_m^*$ that satisfies the normal equations (1.9).

It is clear from the definitions

$$A\mathcal{K}_m^* = \operatorname{span}\left\{A^2b, A^3b, \ldots, A^{m+1}b\right\},$$
$$\mathcal{K}_{m+1}^* = \operatorname{span}\left\{Ab, A^2b, \ldots, A^{m+1}b\right\}$$

that $\mathcal{K}_m^* \subset \mathcal{K}_{m+1}^*$ and $A\mathcal{K}_m^* \subset \mathcal{K}_{m+1}^*$. By hypothesis $\dim \mathcal{K}_m^* = \dim \mathcal{K}_{m+1}^* = m$. Therefore,

$$\mathcal{K}_m^* = \mathcal{K}_{m+1}^*. \tag{3.3}$$

It follows from Lemma 3.1 that $\dim A\mathcal{K}_m^* = m$, i.e., $\dim A\mathcal{K}_m^* = \dim \mathcal{K}_{m+1}^* = m$. Therefore,

$$A\mathcal{K}_m^* = \mathcal{K}_{m+1}^*. \tag{3.4}$$

Combining (3.3) and (3.4) shows that

$$A\mathcal{K}_m^* = \mathcal{K}_m^*. \tag{3.5}$$

Since $Ab \in \mathcal{K}_m^*$, it follows from (3.5) that $Ab \in A\mathcal{K}_m^*$. Thus, there is an element $z \in \mathcal{K}_m^*$, such that $Ab = Az$. It follows from $A(b - z) = 0$ that $b - z \in \mathcal{N}(A)$. By hypothesis, $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$, and therefore

$$A^{\mathrm{T}}(b - z) = 0. \tag{3.6}$$

Since $z \in \mathcal{K}_m^*$, it follows from (3.5) that $z \in A\mathcal{K}_m^*$. Therefore, there is an element $w \in \mathcal{K}_m^*$, such that $z = Aw$. Substituting $z = Aw$ into (3.6) shows that w is a least-squares solution of (1.1). Since, in addition, $w \in \mathcal{R}(A) = \mathcal{N}(A)^\perp$, w is the minimal-norm solution. □

The theorem shows that when the matrix is range symmetric and the RRGMRES method breaks down, the minimal norm least-squares solution has been determined.

Range symmetric matrices are rather special. We will now show that the RRGMRES method also can be applied successfully in more general situations. The following result shows that under suitable conditions the RRGMRES method determines a least-squares solution of the linear system (1.1) even when the matrix A is not range symmetric.

Theorem 3.3. *Apply the RRGMRES method to the inconsistent system* (1.1) *until breakdown at step m. If* $\operatorname{rank}(A) = m - 1$, *then the RRGMRES method produces a least-squares solution of* (1.1).

Proof. The result can be shown similarly as Theorem 2.2. □

Example 3.1. Let A, b and x_0 be defined as in Example 2.1. The RRGMRES method breaks down at step 1 and gives the least-squares solution $x_1 = (1/6, 1/6)^{\mathrm{T}}$.

Theorems 2.2 and 3.3 show that under similar conditions, both the GMRES and RRGMRES methods determine a least-squares solution. We will now consider a situation when the RRGMRES method generally is preferable. Assume that

$$\|Ab\| \ll \|b\|. \tag{3.7}$$

Then very ill-conditioned matrices $\bar{H}_k$ are produced by Arnoldi's method (Algorithm 1.1) and the minimization problems (1.6) are ill-conditioned. This has the effect that the (standard) GMRES method produces approximate solutions x_m of large norm.

The RRGMRES method avoids ill-conditioning due to (3.7) by starting Algorithm 1.1 with the vector Ab, and the initial matrices $\bar{H}_k$ computed are typically much better conditioned than those generated by the standard GMRES method.

Example 3.2. We construct $A \in \mathbb{R}^{100\times 100}$ as follows. Let $D \in \mathbb{R}^{100\times 100}$ be a diagonal matrix, with 75 uniformly distributed random diagonal entries in the interval $[-1, 1]$ and 25 zero diagonal entries. Let $S \in \mathbb{R}^{100\times 100}$ be a random matrix with uniformly distributed random entries in $[-1, 1]$. Define $A = SDS^{-1}$. Let the right-hand side b be such that $\|Ab\|/\|b\| = 1 \cdot 10^{-6}$.

Fig. 1 compares the norm of the approximate solutions x_m and associated residual vectors r_m generated by the GMRES and RRGMRES methods. We note that the norm of the approximate solutions computed by the GMRES method for most

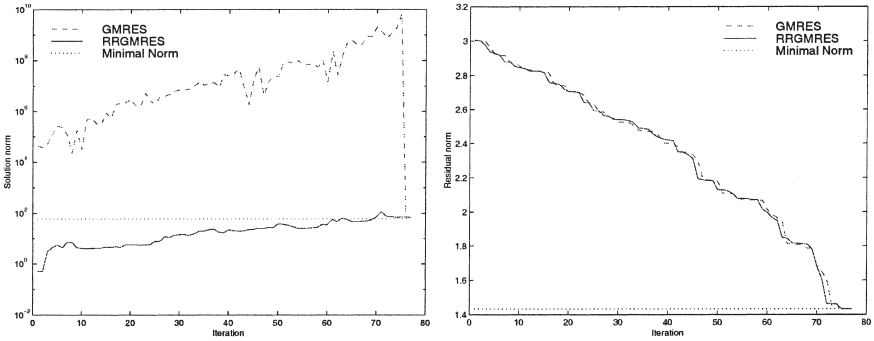

Fig. 1. The GMRES and RRGMRES methods applied to an inconsistent system.

iteration numbers m is much larger than the norm of the corresponding approximate solutions determined by the RRGMRES method.

An implementation of the RRGMRES method can be based on the approach proposed by Walker and Zhou [8] for the implementation of the (standard) GMRES method. They first determine an orthogonal basis of the Krylov space $\mathcal{K}_m^*$ and then append the vector b to obtain a basis for $\mathcal{K}_{m+1}$. We obtain an efficient implementation of the RRGMRES method by generating an orthogonal basis for $\mathcal{K}_m^*$ as described in [8], and then using this basis (without appending b) to solve the minimization problem (3.1). Inspired by the terminology proposed by Walker and Zhou [8], we might refer to the RRGMRES method as "even simpler GMRES".

4. Bounds for the minimal norm least-squares solution

We present two kinds of bounds for the minimal norm least-squares solution $x^\dagger$ of the linear system (1.1). The first bound, formula (4.1) below, bounds the distance between $x^\dagger$ and any other least-squares solution of (1.1). This bound is of interest when we know that the GMRES or RRGMRES methods have determined a least-squares solution; cf. Theorems 2.2 and 3.3. The other bounds of this section determine the distance between $x^\dagger$ and iterates x_m computed by the GMRES or RRGMRES methods. Here the iterates x_m do not have to be least-squares solutions of (1.1). The latter bounds are analogous to bounds recently derived by Hochbruck and Lubich [5].

Proposition 4.1. *Let x be an arbitrary least-squares solution of* (1.1) *and let $x^\dagger$ denote the least-squares solution of minimal norm. Then $x^\dagger - x \in \mathcal{N}(A)$.*

Proof. Partition the least-squares solution x of (1.1) according to $x = y + z$, where $y \in \mathcal{R}(A^T)$ and $z \in \mathcal{N}(A)$, cf. (3.2). The fact that x satisfies the normal equations implies that y satisfies the normal equations,

$$A^{\mathrm{T}}b = A^{\mathrm{T}}Ax = A^{\mathrm{T}}A(y+z) = A^{\mathrm{T}}Ay,$$

and therefore y is a least-squares solution of (1.1). Since $y \in \mathscr{R}(A^{\mathrm{T}})$, it follows that $y = x^{\dagger}$. □

Let $P_{\mathscr{N}(A)}$ denote the orthogonal projection from $\mathbb{R}^n$ to $\mathscr{N}(A)$ and let x_m be a least-squares solution determined by the GMRES or RRGMRES methods. Then Proposition 4.1 yields

$$\|x^{\dagger} - x_m\| = \|P_{\mathscr{N}(A)}x_m\|. \tag{4.1}$$

The bound (4.1) requires x to be a least-squares solution, but is independent of how x has been computed. We now present bounds for the iterates determined by the RRGMRES method. These iterates do not have to be least-squares solutions of (1.1).

Theorem 4.2. *Let x_m be the m*th *iterate generated by the RRGMRES method applied to the linear system* (1.1) *and let $x^{\dagger}$ be the minimal norm least-squares solution of* (1.1). *Then*

$$\|x^{\dagger} - P_{\mathscr{R}(A^{\mathrm{T}})}x_m\| \leqslant \|A^{\dagger}B_m\| \min_{p \in \Pi_m^{(0,1)}} \|p(A)b\|, \tag{4.2}$$

where $A^{\dagger}$ denotes the Moore–Penrose pseudoinverse of A and $\Pi_m^{(0,1)}$ denotes the set of polynomials p of degree at most m, such that $p(0) = 1$ and $p'(0) = 0$, and $P_{\mathscr{R}(A^{\mathrm{T}})}$ denotes the orthogonal projection from $\mathbb{R}^n$ to $\mathscr{R}(A^{\mathrm{T}})$. Let the matrix B_m be a projection of the form

$$B_m = I - V_{m+1}\bar{H}_m\bar{H}_m^{\dagger}V_{m+1}^{\mathrm{T}} \tag{4.3}$$

or

$$B_m = I - V_m H_m H_m^{\dagger} V_m^{\mathrm{T}}, \tag{4.4}$$

where the matrices in (4.3) *are given by the Arnoldi decomposition* (1.5) *with initial vector $V_{m+1}e_1 = Ab/\|Ab\|$. This form of B_m is appropriate when the decomposition* (1.5) *exists. The matrices in* (4.4) *are given by the Arnoldi decomposition* (1.4) *with initial vector $V_m e_1 = Ab/\|Ab\|$. This form of B_m is appropriate when the decomposition* (1.4) *is available with $f_m = 0$.*

Proof. The proof is a modification of the proof for nonsingular matrices A presented in [5]. Let B_m be of the form (4.3). Then

$$\begin{aligned} B_m A V_m &= \left(I - V_{m+1}\bar{H}_m\bar{H}_m^{\dagger}V_{m+1}^{\mathrm{T}}\right) A V_m \\ &= A V_m - V_{m+1}\bar{H}_m\bar{H}_m^{\dagger}\bar{H}_m \\ &= V_{m+1}\bar{H}_m - V_{m+1}\bar{H}_m \\ &= 0. \end{aligned}$$

Using this result and the fact that $P_{\mathscr{R}(A^{\mathrm{T}})} = A^{\dagger}A$, we obtain

$$x^\dagger - P_{\mathscr{R}(A^{\mathrm{T}})}x_m = A^\dagger b - A^\dagger A V_m \bar{H}_m^\dagger V_{m+1}^{\mathrm{T}} b = A^\dagger \left(I - A V_m \bar{H}_m^\dagger V_{m+1}^{\mathrm{T}} \right) b$$
$$= A^\dagger \left(I - V_{m+1} \bar{H}_m \bar{H}_m^\dagger V_{m+1}^{\mathrm{T}} \right) b = A^\dagger B_m b$$
$$= A^\dagger B_m (b - A V_m z) \quad \text{for arbitrary } z \in \mathbb{R}^m. \tag{4.5}$$

We remark that $b - AV_m z = p_m(A)b$ for some polynomial $p_m \in \Pi_m^{(0,1)}$. Conversely, for any polynomial $p_m \in \Pi_m^{(0,1)}$, $p_m(A)b$ can be expressed as $b - AV_m z$ for some $z \in \mathbb{R}^m$. Taking norms in (4.5) gives the desired result. The proof when B_m is of the form (4.4) proceeds similarly. □

A bound analogous to (4.2) has been shown by Hochbruck and Lubich [5] when the iterates are computed by the (standard) GMRES method and the matrix A is nonsingular. An analogue of Theorem 4.2 for the (standard) GMRES method when applied to inconsistent systems also can be formulated. Then the set $\Pi_m^{(0,1)}$ in Theorem 4.2 is replaced by the set $\Pi_m^{(0)}$ consisting of all polynomials p of degree at most m normalized so that $p(0) = 1$, and $V_k e_1 = b/\|b\|$.

When the matrix A is range symmetric, i.e., when $P_{\mathscr{R}(A^{\mathrm{T}})} = P_{\mathscr{R}(A)}$, the bound (4.2) of Theorem 4.2 can be strengthened. Since the iterates x_m computed by RRGMRES are in the range of A, the bound (4.2) then can be written as

$$\|x^\dagger - x_m\| \leqslant \|A^\dagger B_m\| \min_{p \in \Pi_m^{(0,1)}} \|p(A)b\|.$$

5. Application to overdetermined systems

This section presents a computed example in which the GMRES and RRGMRES methods are applied to determine a least-squares solution of an overdetermined inconsistent system of equations

$$\tilde{A}\tilde{x} = b, \quad \tilde{A} \in \mathbb{R}^{n \times m},\ n > m,\ \tilde{x} \in \mathbb{R}^m,\ b \in \mathbb{R}^n. \tag{5.1}$$

The example illustrates that a least-squares solution can be computed without using the transpose of the matrix A by the GMRES and RRGMRES methods, provided that these methods do not break down too early.

The GMRES and RRGMRES methods are defined for square matrices only. We therefore append $n - m$ zero columns to $\tilde{A}$ to obtain the matrix

$$A = \begin{bmatrix} \tilde{A} & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}. \tag{5.2}$$

Introduce $x^{\mathrm{T}} = [\tilde{x}^{\mathrm{T}}, x_{\mathscr{N}}^{\mathrm{T}}]$, where $x_{\mathscr{N}} \in \mathbb{R}^{n-m}$. Then the system (5.1) can be written in the form (1.1) and the GMRES and RRGMRES methods can be applied to its solution. If the columns of $\tilde{A}$ are linearly independent, then $\mathscr{N}(A) = n - m$, and by Theorems 2.2 and 3.3 the GMRES and RRGMRES algorithms determine a least-squares solution of (1.1) and (5.1) if they do not break down until step $m + 1$.

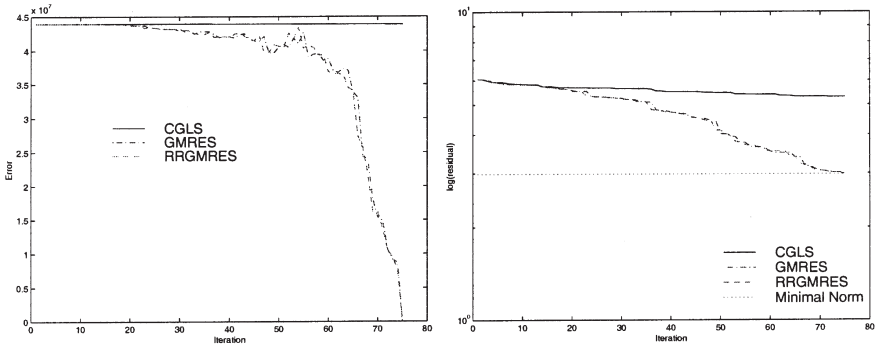

Fig. 2. The GMRES, RRGMRES and CGLS methods applied to an overdetermined system.

Example 5.1. Let the matrix $A \in \mathbb{R}^{100\times 75}$ be defined as follows. Introduce $D = [d_{i,j}] \in \mathbb{R}^{100\times 75}$, where $d_{i,i} = i^{-4}$ and $d_{i,j} = 0$ for $i \neq j$. Let $U \in \mathbb{R}^{100\times 100}$ and $V \in \mathbb{R}^{75\times 75}$ be random orthonormal matrices generated by applying the *QR* factorization to matrices with uniform random entries in $[0, 1]$. Let $A = UDV$. Then the condition number of A as measured by $d_{1,1}/d_{75,75}$ is $3 \cdot 10^7$. Let the right-hand side vector be $b = (1, 1, \ldots, 1)^{\mathrm{T}}$.

Fig. 2 displays iterates and residual errors determined by the GMRES and RRGMRES methods. For comparison, we also solve the system (5.1) by the conjugate gradient method applied to the normal equations. We use the CGLS algorithm described by Björck [2, Chapter 7] for this purpose. Denote the iterates generated by the different methods by x_m and the associated residuals by r_m. Fig. 2 shows the quantity $\|x^{\dagger} - x_m\|$ (referred to as error) and the 10-logarithm of the norm of the residual vectors $\|r_m\|$ for the different iteration methods as a function of the iteration number m. Note that the CGLS algorithm does not converge within 75 iterations.

6. Conclusion

The paper sheds light on the behavior of GMRES-like methods when applied to inconsistent linear systems of equations. The RRGMRES method, which restricts the computed approximate solution to the range of A, is found to be well suited for the solution of inconsistent linear systems.

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