

BREAKDOWN-FREE GMRES FOR SINGULAR SYSTEMS*

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Abstract. GMRES is a popular iterative method for the solution of large linear systems of equations with a square nonsingular matrix. When the matrix is singular, GMRES may break down before an acceptable approximate solution has been determined. This paper discusses properties of GMRES solutions at breakdown and presents a modification of GMRES to overcome the breakdown.

Key words. iterative method, Krylov subspace, singular matrix, linear system

AMS subject classifications. 65F10, 65F20

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1. Introduction. GMRES by Saad and Schultz [17] is one of the most popular methods for the iterative solution of large nonsymmetric linear systems of equations

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

The performance of the method is well understood when A is nonsingular, but the method also can be applied when A is singular. This paper focuses on the latter case. For notational simplicity, we choose the initial approximate solution of (1.1) to be $x_0 := 0$ and assume that the right-hand side vector b in (1.1) is normalized so that $\|b\| = 1$. Here and throughout this paper $\|\cdot\|$ denotes the Euclidean vector norm or the associated induced matrix norm.

The standard implementation of GMRES is based on the Arnoldi process. Application of k steps of the Arnoldi process to the matrix A with initial vector b yields the Arnoldi decomposition

$$(1.2) \quad AV_k = V_k H_k + f_k e_k^T,$$

where $H_k \in \mathbb{R}^{k \times k}$ is an upper Hessenberg matrix, $V_k \in \mathbb{R}^{n \times k}$, $V_k e_1 = b$, $V_k^T V_k = I_k$, $V_k^T f_k = 0$, I_k denotes the identity matrix of order k , and e_k is the k th axis vector. When $f_k \neq 0$, it is convenient to define the matrices

$$(1.3) \quad V_{k+1} := \begin{bmatrix} V_k & \frac{f_k}{\|f_k\|} \end{bmatrix} \in \mathbb{R}^{n \times (k+1)}, \quad \hat{H}_k := \begin{bmatrix} H_k & \\ \|f_k\| e_k^T \end{bmatrix} \in \mathbb{R}^{(k+1) \times k}$$

and express (1.2) in the form

$$(1.4) \quad AV_k = V_{k+1} \hat{H}_k.$$

Note that $V_{k+1}^T V_{k+1} = I_{k+1}$. We assume that k is small enough so that at least one of the Arnoldi decompositions (1.2) or (1.4) exists. We will comment on the size of k below.

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It follows from (1.2) and the orthonormality of the columns of V_k that the latter form an orthonormal basis of the Krylov subspace

$$\mathcal{K}_k(A, b) := \text{span}\{b, Ab, \dots, A^{k-1}b\}.$$

We will write \mathcal{K}_k instead of $\mathcal{K}_k(A, b)$ when there is no ambiguity.

The k th iterate, x_k , determined by GMRES satisfies

$$\|b - Ax_k\| = \min_{z \in \mathcal{K}_k} \|b - Az\|, \quad x_k \in \mathcal{K}_k.$$

Assuming that $f_k \neq 0$, the iterate x_k is computed by first solving the minimization problem in the right-hand side of

$$(1.5) \quad \min_{z \in \mathcal{K}_k} \|b - Az\| = \min_{y \in \mathbb{R}^k} \|b - AV_k y\| = \min_{y \in \mathbb{R}^k} \|e_1 - \hat{H}_k y\|$$

for $y_k \in \mathbb{R}^k$. Then x_k is given by

$$(1.6) \quad x_k := V_k y_k.$$

Since the subdiagonal entries of \hat{H}_k are nonvanishing, the matrix \hat{H}_k is of full rank, and therefore y_k is uniquely determined. We refer to Saad [16] and Saad and Schultz [17] for implementation details.

We say that the Arnoldi process (1.2) breaks down at step k if $f_k = 0$. Then the minimization problem (1.5) can be expressed as

$$(1.7) \quad \min_{z \in \mathcal{K}_k} \|b - Az\| = \min_{y \in \mathbb{R}^k} \|b - AV_k y\| = \min_{y \in \mathbb{R}^k} \|e_1 - H_k y\|,$$

and the solution y_k of the minimization problem in the right-hand side yields the solution $x := V_k y_k$ of (1.1). In this case, it is easy to show that if A is nonsingular, then H_k is nonsingular and y_k is uniquely determined.

When the matrix A is singular, the Arnoldi process may break down at step k with the upper Hessenberg matrix H_k in the decomposition (1.2) being singular. Let y_k denote the least-squares solution of minimal Euclidean norm of the minimization problem on the right-hand side of (1.7). The vector $x_k := V_k y_k$ is not guaranteed to solve the linear system of equations (1.1). The investigations [4, 5, 8] shed light on the properties of x_k , specifically on the question of whether x_k is a least-squares solution of (1.1). Related results also can be found in the review [14]. Several Krylov subspace methods for nonsymmetric singular systems are described in [1, 10, 11, 12, 18]. The present paper focuses on GMRES. Singular systems, several generalized inverses, and their applications are discussed in [2, 9].

We say that GMRES breaks down at step k if the Arnoldi process breaks down at step k . In this paper, we first discuss various properties of GMRES at breakdown, such as whether a solution is contained in the Krylov subspace and hence found by GMRES, and if not, what subspace contains a solution. Both consistent and inconsistent systems are considered. We then introduce a generalization of the Arnoldi decomposition that can be used when the (standard) Arnoldi process breaks down. We refer to GMRES based on the generalized Arnoldi decomposition as *breakdown-free GMRES* or simply *BFGMRES*. We also describe a breakdown-free variant of range restricted GMRES, which we refer to as *BFRRGMRES*. The (standard) RRGMRRES method was introduced in [5]. Our interest in RRGMRRES stems from the fact that

the method can determine more accurate approximations of the desired solution of large-scale discrete ill-posed problems than GMRES can; see [6] for illustrations. We remark that our approach to overcome breakdown of the Arnoldi process is related to but quite different from the technique described in [19] for avoiding breakdown of the nonsymmetric Lanczos process.

This paper is organized as follows. Section 2 discusses properties of approximate solutions determined by GMRES at breakdown when applied to the solution of consistent and inconsistent linear systems of equations with a singular matrix. Section 3 presents an algorithm for BFGMRES and discusses the minor modification required to obtain an algorithm for BFRRGMRES. Some properties of (BF)RRGMRES are also discussed. A few numerical examples are presented in section 4.

We remark that linear systems of equations with a numerically singular matrix arise, for instance, in the context of ill-posed problems (see [6, 7]) and when computing the steady state distribution of finite Markov chains; see, e.g., [15]. Furthermore, overdetermined systems of equations with n rows and m columns, where $n > m$, can be brought into the form (1.1) by appending $n - m$ zero columns to the matrix. The matrix A so obtained is singular, and the linear system of equations can be solved by BFGMRES or BFRRGMRES. A comparison of this approach with application of the conjugate gradient method to the normal equations is presented in section 4. Underdetermined linear systems of equations can also be solved by BFGMRES or BFRRGMRES by first appending an appropriate number of zero rows to the matrix.

2. Breakdown of GMRES. We first discuss breakdown of the (standard) Arnoldi process in some detail and introduce the notions of benign and hard breakdowns. There is a positive integer N , such that

$$\dim(\mathcal{K}_k) = \begin{cases} k, & 1 \leq k \leq N, \\ N, & k \geq N + 1. \end{cases}$$

This easily can be seen by using the Jordan form of A . Clearly, $N \leq n$.

For $k \leq N$, the Arnoldi decomposition (1.2) exists. We distinguish two cases:

1. If $Av_k \notin \mathcal{K}_k$, then $f_k \neq 0$ in (1.2). It follows that the decomposition (1.4) exists, and the columns of the matrix V_{k+1} form an orthonormal basis of \mathcal{K}_{k+1} , the matrix \tilde{H}_k is of full rank, and the minimization problem in the right-hand side of (1.5) has a unique solution y_k , which by (1.6) determines x_k , the k th iterate generated by GMRES. It follows from $\dim(\mathcal{K}_{k+1}) = k + 1$ that $Ax_k \neq b$.
2. If $Av_k \in \mathcal{K}_k$, then $f_k = 0$ in the Arnoldi decomposition (1.2). We have $\dim(\mathcal{K}_{k+1}) = k$, and therefore $k = N$. The Arnoldi process and GMRES break down. Again, we distinguish two cases:
 - (a) If $\dim(A\mathcal{K}_N) = N$, then $\text{rank}(H_N) = N$, and the N th iterate, x_N , generated by GMRES is determined by first solving the minimization problem in the right-hand side of (1.7), with k replaced by N , for y_N , and then computing x_N from (1.6) with k replaced by N . Since

$$\text{span}\{b\} + A\mathcal{K}_N = \mathcal{K}_{N+1}, \quad \dim(\mathcal{K}_{N+1}) = N,$$

we have that $b \in A\mathcal{K}_N$. Thus, $Ax_N = b$. Therefore, this is referred to as a *benign breakdown*; the solution has been found when the breakdown occurs, just like when the matrix A is nonsingular.

- (b) If $\dim(A\mathcal{K}_N) < N$, then $\text{rank}(H_N) < N$. Let y_N be the solution of minimal norm of the least-squares problem in the right-hand side of

(1.7), and determine the iterate x_N by (1.6) with k replaced by N . Note that $Ax_N \neq b$ because $b \notin AK_N$. We refer to this as a *hard breakdown*.

We remark that our classification of breakdowns is slightly different from that of Brown and Walker [4].

Next, we characterize the approximate solutions of (1.1) that can be determined by GMRES when a hard breakdown occurs. Throughout this paper $\mathcal{N}(M)$ denotes the null space and $\mathcal{R}(M)$ denotes the range of the matrix M . We consider consistent and inconsistent systems separately.

2.1. Consistent systems. Ipsen and Meyer [14] showed that Krylov subspace iterative methods, such as GMRES, are able to determine a solution of the linear system of equations (1.1) if and only if $b \in \mathcal{R}(A^D)$, where A^D denotes the Drazin inverse of A ; see (2.10) below for a definition. The following theorem complements this result; it discusses the form of the solution when the right-hand side b is a general vector in $\mathcal{R}(A)$.

THEOREM 2.1. *Let the matrix A be singular and assume that the linear system of equations (1.1) is consistent. Apply GMRES with initial approximate solution $x_0 := 0$ to the solution of (1.1) and assume that a hard breakdown occurs at step N . If $A^N b \neq 0$, then any solution x of (1.1) can be expressed as*

$$(2.1) \quad x = \hat{x} + u,$$

where $\hat{x} \in \mathcal{K}_{N-1}$ and $u \in \mathcal{N}(A^\ell) \setminus \{0\}$ for some integer ℓ with $2 \leq \ell \leq N$. If instead $A^N b = 0$, then any solution of (1.1) belongs to $\mathcal{N}(A^{N+1})$.

Proof. We first consider the case when $A^N b \neq 0$. Since $\dim(\mathcal{K}_N) = N$ and $\dim(A\mathcal{K}_N) < N$, the vector $A^N b$ is a linear combination of the vectors $\{A^j b\}_{j=1}^{N-1}$. Let ℓ be the largest integer with $2 \leq \ell \leq N$, such that

$$(2.2) \quad \alpha_{\ell-1} A^{\ell-1} b + \alpha_\ell A^\ell b + \cdots + \alpha_{N-1} A^{N-1} b + A^N b = 0$$

for some coefficients $\alpha_{\ell-1}, \alpha_\ell, \dots, \alpha_{N-1}$. Clearly, $\alpha_{\ell-1} \neq 0$.

Let x be a solution of (1.1). Then (2.2) yields

$$A^\ell x + \frac{\alpha_\ell}{\alpha_{\ell-1}} A^\ell b + \cdots + \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-1} b + \frac{1}{\alpha_{\ell-1}} A^N b = 0$$

or, equivalently,

$$(2.3) \quad A^\ell \left(x + \frac{\alpha_\ell}{\alpha_{\ell-1}} b + \cdots + \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell-1} b + \frac{1}{\alpha_{\ell-1}} A^{N-\ell} b \right) = 0.$$

Let

$$\hat{x} := -\frac{\alpha_\ell}{\alpha_{\ell-1}} b - \cdots - \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell-1} b - \frac{1}{\alpha_{\ell-1}} A^{N-\ell} b, \quad u := x - \hat{x}.$$

Clearly, $\hat{x} \in \mathcal{K}_{N-\ell+1} \subset \mathcal{K}_{N-1}$, and it follows from (2.3) that $u \in \mathcal{N}(A^\ell)$. Since $A\hat{x} \neq b$, we have $u \neq 0$.

We turn to the case when $A^N b = 0$. With $b = Ax$, we have $A^{N+1}x = 0$, which shows that $x \in \mathcal{N}(A^{N+1})$. \square

The matrix A is said to have index p if its largest Jordan block associated with the eigenvalue zero is of order p . It follows that if A has index p , then $\mathcal{N}(A^j) = \mathcal{N}(A^p)$

for all integers $j \geq p$. Then by Theorem 2.1 any solution x belongs to a subspace extended from the Krylov subspace, i.e.,

$$(2.4) \quad x \in \mathcal{K}_{N-1} + \mathcal{N}(A^p).$$

We note that only the Krylov subspace \mathcal{K}_{N-1} is needed. This is different from the situation of benign breakdown, where the solution of (1.1) belongs to \mathcal{K}_N . This fact will be used in our extension of GMRES described in section 3.

Brown and Walker [4, Theorem 2.6] show that if the linear system of equations (1.1) is consistent and

$$(2.5) \quad \mathcal{N}(A) \cap \mathcal{R}(A) = \{0\},$$

then GMRES applied to (1.1) with initial approximate solution $x_0 := 0$ determines a solution. This result is a corollary to the theorem above. Note that condition (2.5) is equivalent to A having index one.

COROLLARY 2.2. *Let A be a singular matrix of index one, and assume that the linear system of equations (1.1) is consistent. Then hard breakdown cannot occur.*

Proof. We use the notation of Theorem 2.1 and its proof. Assume that a hard breakdown occurs at step N of GMRES. First consider the situation when $A^N b \neq 0$. Theorem 2.1 shows that $\hat{x} = x - u$ with $u \in \mathcal{N}(A^\ell) = \mathcal{N}(A)$. Therefore, $A\hat{x} = Ax - Au = b$, which is a contradiction.

We turn to the case when $A^N b = 0$ and $b \neq 0$. Then $x \in \mathcal{N}(A^{N+1}) = \mathcal{N}(A)$. Hence, $Ax = 0$, which is a contradiction. \square

We consider an application of Corollary 2.2.

Example 2.1. Let $\tilde{A} \in \mathbb{R}^{n \times \ell}$, with $\ell < n$, and assume that the leading $\ell \times \ell$ principal submatrix of \tilde{A} is nonsingular. Let $b \in \mathcal{R}(\tilde{A})$. We are interested in computing the solution of the consistent linear system of equations

$$(2.6) \quad \tilde{A}\tilde{x} = b.$$

Assume that a function for the evaluation of matrix-vector products with the matrix \tilde{A} is available, but that the entries of the matrix are not explicitly known. It then may be attractive to solve (2.6) by an iterative method. The standard iterative method for this task is the conjugate gradient method applied to the normal equations associated with (2.6), using the CGLS or LSQR algorithms; see, e.g., [3]. These algorithms require the evaluation of matrix-vector products with both the matrices \tilde{A} and \tilde{A}^T . If only a function for the evaluation of matrix-vector products with \tilde{A} is available, but not with \tilde{A}^T , then we may consider using GMRES, which does not require \tilde{A}^T . We note that the cost per iteration for GMRES increases rapidly with the iteration and restarts are needed in practical implementations. The fact that the matrix \tilde{A} is not square can be overcome by padding \tilde{A} with $n - \ell$ trailing zero columns. This yields an $n \times n$ matrix, which we denote by A , and we obtain a linear system of equations of the form (1.1). GMRES then is applied to compute an approximate solution of this system. Note that zero is an eigenvalue of A of algebraic multiplicity $n - \ell$; this can be seen from the Schur form. Moreover, the axis vectors $e_{\ell+1}, e_{\ell+2}, \dots, e_n$ are in $\mathcal{N}(A)$. It follows that A has index one, and by Corollary 2.2, GMRES cannot suffer from a hard breakdown.

Let $x_k \in \mathbb{R}^n$ denote the k th iterate determined by GMRES. The first ℓ entries of x_k yield an approximate solution of (2.6). The zero columns of A , of course, do not have to be stored.

We remark that the requirement that \tilde{A} have a nonsingular $\ell \times \ell$ leading principal submatrix secures that the matrix is of full rank. Conversely, if \tilde{A} is of full rank, then there is a row-permutation such that the leading principal $\ell \times \ell$ submatrix is nonsingular. We also observe that different row permutations could lead to a very different performance of GMRES, because the spectrum of A may change as the rows are interchanged. A comparison of the convergence behavior of CGLS and GMRES when applied to the solution of linear systems of equations of the form (2.6) is presented in section 4.

We also consider the special case when a breakdown occurs when the dimension of the Krylov subspace N is equal to the rank of A . This should be compared with Theorem 2.7 below where interestingly a much stronger result exists for inconsistent systems.

THEOREM 2.3. *Let the matrix $A \in \mathbb{R}^{n \times n}$ be of rank $N < n$ and assume that the linear system of equations (1.1) is consistent. Apply GMRES with initial approximate solution $x_0 := 0$ to the solution of (1.1). Assume that GMRES breaks down at step N . If $\dim(AK_N) = N$, then GMRES determines a solution of (1.1) at breakdown. If, instead, $\dim(AK_N) < N$, then (1.1) has a solution in $K_N + \mathcal{R}(A^T)$.*

Proof. The Arnoldi process breaks down at step N and yields the decomposition

$$(2.7) \quad AV_N = V_N H_N, \quad V_N e_1 = b.$$

If $\dim(AK_N) = N$, then the breakdown is benign and GMRES determines a solution of (1.1).

We turn to the case when $\dim(AK_N) < N$. Then the upper Hessenberg matrix H_N in the decomposition (2.7) is singular. Since H_N has positive subdiagonal entries, $\text{rank}(H_N) = N - 1$. Let $u \in \mathcal{N}(H_N^T)$ be of unit length and introduce $v := A^\dagger V_N u$, where A^\dagger denotes the Moore–Penrose pseudoinverse of A . Note that $v \in \mathcal{R}(A^T)$. Since $b \in \mathcal{R}(A)$, we have that $\mathcal{R}(V_N) \subset \mathcal{R}(A)$. Therefore, $Av = V_N u$ and it follows that $V_N^T Av = u$. We seek a solution of (1.1) of the form

$$x = V_N y + v\eta, \quad y \in \mathbb{R}^N, \quad \eta \in \mathbb{R}.$$

Substituting this expression into (1.1) yields the equation $AV_N y + Av\eta = b$, which, using (2.7), can be seen to be equivalent to

$$(2.8) \quad [H_N, u] \begin{bmatrix} y \\ \eta \end{bmatrix} = e_1.$$

Since the matrix $[H_N, u] \in \mathbb{R}^{N \times (N+1)}$ is of full rank, (2.8) has a solution $\{\hat{y}, \hat{\eta}\}$, which gives the solution $\hat{x} := V_N \hat{y} + v\hat{\eta}$ of (1.1). \square

In the second case of the theorem, i.e., when $\dim(AK_N) < N$, a solution of (1.1) can be determined by a modification of GMRES that minimizes the residual error over $K_N + \mathcal{R}(A^T)$.

2.2. Inconsistent systems. First, we note that, for inconsistent systems, H_N in the Arnoldi decomposition determined at breakdown must be singular, because otherwise a solution to (1.1) would be obtained. Therefore, only hard breakdown can occur. We consider the computation of a least-squares solution of (1.1) and formulate our results in terms of the Drazin inverse of A . Let A have the representation

$$(2.9) \quad A = C \begin{bmatrix} J_0 & 0 \\ 0 & J_1 \end{bmatrix} C^{-1},$$

where the matrix $C \in \mathbb{C}^{n \times n}$ is invertible, the matrix J_0 consists of all Jordan blocks associated with the eigenvalue zero, and the matrix J_1 consists of all Jordan blocks associated with nonvanishing eigenvalues. The Drazin inverse of A is given by

$$(2.10) \quad A^D := C \begin{bmatrix} 0 & 0 \\ 0 & J_1^{-1} \end{bmatrix} C^{-1}.$$

See [9, Chapter 7] for properties of this generalized inverse. We note that if A has index p , then

$$\mathcal{N}(A^p) = \mathcal{N}(A^D).$$

THEOREM 2.4. *Let the singular matrix A have index p . Assume that a hard breakdown occurs at step N when GMRES is applied to (1.1) with initial approximate solution $x_0 := 0$, and that $A^N b \neq 0$. Then any least-squares solution x of (1.1) can be written in the form*

$$(2.11) \quad x = \hat{x} + u - A^D r,$$

where $\hat{x} \in \mathcal{K}_{N-1}$, $u \in \mathcal{N}(A^D) = \mathcal{N}(A^p)$, and $r := b - Ax \in \mathcal{N}(A^T)$ is the residual vector associated with x .

Proof. Similarly as in the proof of Theorem 2.1, let ℓ be the largest integer with $2 \leq \ell \leq N$, such that (2.2) holds. It follows that

$$A^{\ell-1} \left(b + \frac{\alpha_\ell}{\alpha_{\ell-1}} Ab + \cdots + \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell} b + \frac{1}{\alpha_{\ell-1}} A^{N-\ell+1} b \right) = 0.$$

Since $\mathcal{N}(A^{\ell-1}) \subset \mathcal{N}(A^p)$, we also have

$$(2.12) \quad A^p \left(b + \frac{\alpha_\ell}{\alpha_{\ell-1}} Ab + \cdots + \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell} b + \frac{1}{\alpha_{\ell-1}} A^{N-\ell+1} b \right) = 0.$$

Let x be a least-squares solution of (1.1) and introduce the associated residual vector $r := b - Ax$. Substituting $b = r + Ax$ into (2.12) yields

$$A^p \left(Ax + \frac{\alpha_\ell}{\alpha_{\ell-1}} Ab + \cdots + \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell} b + \frac{1}{\alpha_{\ell-1}} A^{N-\ell+1} b \right) = -A^p r,$$

and, therefore,

$$(2.13) \quad A^{p+1} \left(x + \frac{\alpha_\ell}{\alpha_{\ell-1}} b + \cdots + \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell-1} b + \frac{1}{\alpha_{\ell-1}} A^{N-\ell} b \right) = -A^p r.$$

Let

$$\hat{x} := -\frac{\alpha_\ell}{\alpha_{\ell-1}} b - \cdots - \frac{\alpha_{N-1}}{\alpha_{\ell-1}} A^{N-\ell-1} b - \frac{1}{\alpha_{\ell-1}} A^{N-\ell} b, \quad w := x - \hat{x}.$$

Then $\hat{x} \in \mathcal{K}_{N-\ell+1} \subset \mathcal{K}_{N-1}$ and

$$(2.14) \quad A^{p+1} w = -A^p r.$$

The linear system of equations (2.14) is consistent, and any solution can be expressed as $w = -A^D r + u$, where A^D denotes the Drazin inverse of A and $u \in \mathcal{N}(A^p)$. We remark that $\mathcal{R}(A^D) + \mathcal{N}(A^D)$ makes up all of the n -space. \square

The following corollary considers the situation when, in addition to the conditions of Theorem 2.4,

$$(2.15) \quad \mathcal{N}(A^T) \subset \mathcal{N}(A^D).$$

In this case, the following result, which is similar to our result for the consistent case, holds.

COROLLARY 2.5. *Let the singular matrix A have index p and assume that a hard breakdown occurs at step N when GMRES is applied to (1.1) with initial approximate solution $x_0 := 0$. Let x be a least-squares solution of (1.1) and assume that (2.15) holds. If $A^N b \neq 0$, then x can be written in the form*

$$(2.16) \quad x = \hat{x} + u,$$

where $\hat{x} \in \mathcal{K}_{N-1}$ and $u \in \mathcal{N}(A^D) = \mathcal{N}(A^p)$. If, instead, $A^N b = 0$, then $x \in \mathcal{N}(A^D)$.

Proof. First assume that $A^N b \neq 0$. Let $r := b - Ax$ denote the residual vector associated with the least-squares solution x of (1.1). Then $r \in \mathcal{N}(A^T)$ and (2.15) yields $A^D r = 0$. Equation (2.16) now follows from (2.11).

If $A^N b = 0$, then $A^p b = 0$. Therefore,

$$0 = A^p b = A^p(r + Ax) = A^p r + A^{p+1}x = A^{p+1}x,$$

and $x \in \mathcal{N}(A^D)$ follows from $\mathcal{N}(A^{p+1}) = \mathcal{N}(A^D)$. \square

Let

$$(2.17) \quad A = QSQ^*$$

be a Schur decomposition; i.e., $S \in \mathbb{C}^{n \times n}$ is upper triangular, $Q \in \mathbb{C}^{n \times n}$ is unitary, and the superscript $*$ denotes transposition and complex conjugation. Order the eigenvalues and partition

$$(2.18) \quad S = \begin{bmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{bmatrix}$$

so that all diagonal entries of S_{11} are zero and the diagonal entries of S_{22} are nonvanishing. Using $\mathcal{N}(A^p) = \mathcal{N}(A^n)$ and $S_{11}^n = 0$, we can show that $S_{11} J_1$ in $S_{11}^p = 0$. $\mathcal{N}(A^T) \subset \mathcal{N}(A^p)$ is equivalent to $\mathcal{N}(S_{11}^T) \subset \mathcal{N}(S_{12}^T)$.

The following result by Brown and Walker [4, Theorem 2.4] can be shown in a similar manner as Theorem 2.4 above. We include a proof for completeness.

COROLLARY 2.6. *Let A be a singular matrix, such that $\mathcal{N}(A) = \mathcal{N}(A^T)$. Apply GMRES to (1.1) with initial approximate solution $x_0 := 0$. Then GMRES determines a least-squares solution at breakdown.*

Proof. Using the Schur decomposition (2.17) of A and the partitioning (2.18), it can be shown that the condition $\mathcal{N}(A^T) = \mathcal{N}(A)$ implies that $S_{11} = 0$ and $S_{12} = 0$. Hence, A has index $p = 1$. Thus, (2.15) holds, and therefore the conditions of Corollary 2.5 are satisfied. Assume that GMRES breaks down at step N . If $A^N b \neq 0$, then Corollary 2.5 shows that a least-squares solution x can be expressed as $x = \hat{x} + u$, where $\hat{x} \in \mathcal{K}_{N-1}$ and $u \in \mathcal{N}(A^p) = \mathcal{N}(A)$. It follows that $b - A\hat{x} = b - Ax$ and, therefore, \hat{x} is a least-squares solution of (1.1). Since GMRES minimizes the Euclidean norm of the residual error over \mathcal{K}_N , GMRES will determine a least-squares solution.

If, instead, $A^N b = 0$, then $Ab = 0$, and therefore $A^T b = 0$. Hence, $x = 0$ is a least-squares solution and so is any multiple of b . GMRES breaks down at step one and yields the least-squares problem

$$(2.19) \quad \min_{y \in \mathbb{R}} |H_1 y - 1|$$

with $H_1 = 0$, where we have used that $\|b\| = 1$. The minimal-norm least-squares solution $y := 0$ gives the least-squares solution $x := 0$ of (1.1). A least-squares solution $y \neq 0$ of (2.19) yields the least-squares solution $x := yb$ of (1.1). \square

Corollary 2.6 holds for any right-hand side vector b in (1.1) but requires that $\mathcal{N}(A) = \mathcal{N}(A^T)$. We remark that GMRES often can find a least-squares solution even when this condition does not hold (see Example 4.1 below). The following result, first stated in [5, Theorem 2.2], explains this observed behavior. It deals with the most typical situation of breakdown, i.e., a breakdown at step $\text{rank}(A) + 1$, which is the upper bound of the dimension of the Krylov subspace as $\mathcal{K}_{k+1} = \text{span}\{b\} + A\mathcal{K}_k$ and $b \notin \mathcal{R}(A)$.

THEOREM 2.7. *Let the matrix $A \in \mathbb{R}^{n \times n}$ be of rank $N < n$ and apply GMRES with initial approximate solution $x_0 := 0$ to the solution of (1.1). If GMRES breaks down at step $N + 1$, then GMRES determines a least-squares solution.*

Proof. An index is incorrect in the proof in [5]; the index is not consistent with the definition of breakdown in [5], which is different from the definition in the present paper. We therefore provide a proof here.

The Arnoldi process generates an orthonormal basis of the Krylov subspace $\mathcal{K}_{N+1} = \text{span}\{b\} + A\mathcal{K}_N$ before breakdown. It follows that $\dim(A\mathcal{K}_N) = N$. Suppose that GMRES does not determine a least-squares solution of (1.1); i.e., there is no $x \in \mathcal{K}_{N+1}$ that satisfies the normal equations $A^T A x = A^T b$. In other words,

$$(2.20) \quad A^T b \notin A^T A \mathcal{K}_{N+1}.$$

By Lemma 2.1 in [5], or by [4, pp. 40–41], $\dim(A^T A \mathcal{K}_{N+1}) = \dim(A\mathcal{K}_{N+1})$, and since $\dim(A\mathcal{K}_{N+1}) \geq \dim(A\mathcal{K}_N) = N$, we obtain that $\dim(A^T A \mathcal{K}_{N+1}) \geq N$. It now follows from (2.20) that $A^T \mathcal{K}_{N+2} = \text{span}\{A^T b\} + A^T A \mathcal{K}_{N+1}$ is of dimension at least $N + 1$. However, $\text{rank}(A^T) = \text{rank}(A) = N$. Therefore, $\dim(A^T \mathcal{K}_{N+2}) \leq N$. This contradiction shows that \mathcal{K}_{N+1} does contain a least-squares solution of the normal equation. Hence, GMRES determines a least-squares solution. \square

The conditions of Theorem 2.7 hold if $p(A)b \neq 0$ for any polynomial p of degree less than or equal to N . This is the case, for example, when A has distinct nonzero eigenvalues, at most one zero eigenvalue with a nontrivial Jordan block, and each eigenvector and its associated Jordan chain have a nonzero component in b . We also note that the conditions can be satisfied only if the linear system (1.1) is inconsistent, because otherwise $\mathcal{R}(V_{N+1}) \subset \mathcal{R}(A)$. But this inclusion cannot hold since $\dim(\mathcal{R}(A)) = N$.

Example 2.2. Let \tilde{A} be a matrix of the same kind as in Example 2.1, and assume that $b \in \mathbb{R}^n$ is not in $\mathcal{R}(A)$. We are interested in computing the solution of the least-squares problem

$$(2.21) \quad \min_{\tilde{x} \in \mathbb{R}^\ell} \|\tilde{A}\tilde{x} - b\|.$$

Similarly as in Example 2.1, we define the matrix $A \in \mathbb{R}^{n \times n}$ by padding \tilde{A} with $n - \ell$ trailing zero columns. We obtain a linear system of equations of the form (1.1). If

GMRES applied to this system with initial approximate solution $x_0 := 0$ does not break down until step $\ell + 1$, then according to Theorem 2.7 a least-squares solution of (1.1) has been determined. The first ℓ components of the computed solution make up a least-squares solution of (1.1).

This example illustrates that it may be possible to determine a solution of (2.21) by (standard) GMRES. The breakdown-free GMRES method of the following section is useful when (standard) GMRES breaks down before step $\ell + 1$.

3. Breakdown-free GMRES. This section presents an extension of GMRES to overcome breakdown. We comment on a breakdown-free variant of RRGMRRES at the end of the section.

From our discussions in section 2, when GMRES suffers a hard breakdown at step N , the Krylov subspace \mathcal{K}_N does not contain a solution of the linear system (1.1); however, as Theorem 2.1 shows, any solution belongs to $\mathcal{K}_{N-1} + \mathcal{N}(A^p)$. This suggests that, to compute a solution, the Krylov subspace \mathcal{K}_{N-1} has to be extended to capture the component of the solution in $\mathcal{N}(A^p)$, which is an eigenvector of A^p corresponding to the eigenvalue zero. This eigenvector can be approximated from a Krylov subspace generated by a new vector. Therefore, at every breakdown of the Arnoldi process, we generate a new Krylov subspace and add it to the available one(s). Then we seek an approximation from the extended subspace. An implementation is presented below.

We remark that our approach for avoiding breakdown is related to but different from the technique for the nonsymmetric Lanczos algorithm presented in [19]. In [19] a new Krylov subspace is appended to the existing Krylov subspace \mathcal{K}_N and both subspaces are expanded after breakdown. In the present paper, we instead append a new Krylov subspace to \mathcal{K}_{N-1} without further expanding \mathcal{K}_{N-1} as follows. Let v_j denote the j th column of the matrix V_k in (1.2); i.e., $V_k = [v_1, v_2, \dots, v_k]$. It follows from (1.3) that if $f_k \neq 0$, then $v_{k+1} = f_k / \|f_k\|$. Moreover, let $h_{i,j}$ denote the entry in position (i, j) of the matrices H_k in (1.2) or \hat{H}_k in (1.4). It follows from (1.3) that $h_{k+1,k} = \|f_k\|$. Identifying the k th column of the right-hand and left-hand sides of (1.4) yields

$$(3.1) \quad Av_k = h_{1,k}v_1 + \dots + h_{k,k}v_k + h_{k+1,k}v_{k+1}.$$

Assume that GMRES breaks down at step N . Then the Arnoldi decomposition (1.2) holds with $k = N$ and $f_N = 0$. If H_N is nonsingular, then GMRES finds the solution of (1.1) at this step. On the other hand, if H_N is singular, then GMRES cannot determine the solution of (1.1).

We remark that an exact breakdown is rare in actual computations in floating-point arithmetic. However, we have to be concerned about near-breakdown when the orthogonal projection of the vector Av_N into the complement of \mathcal{K}_N is nonvanishing but “tiny.” In this situation, we can still determine the last column $v_{N+1} = f_{N+1} / \|f_{N+1}\|$ of the matrix V_{N+1} in the Arnoldi decomposition (1.4), but the entry $h_{N+1,N}$ of \hat{H}_N is tiny. If the matrix \hat{H}_N is well conditioned, then this is a benign near-breakdown, and the computations can be continued with (standard) GMRES. On the other hand, if \hat{H}_N is severely ill conditioned, then we are suffering from a hard near-breakdown, and standard GMRES will have difficulties finding a solution. Theorem 2.1 shows that in case of a hard breakdown at step N , with $A^N b \neq 0$, a component of the solution belongs to $\text{span}\{v_1, v_2, \dots, v_{N-1}\} = \mathcal{K}_{N-1}$, but the column v_N of V_N is not required to represent the solution. We therefore replace this column by a unit vector, say, \hat{v} , which is orthogonal to the columns v_1, v_2, \dots, v_N of V_N . Such a vector can be generated, for example, by orthogonalizing a random vector against

v_1, v_2, \dots, v_N . We also report numerical experiments in which we determine the vector \hat{v} by orthogonalizing $A^T r_{N-1}$ against v_1, v_2, \dots, v_N , where $r_{N-1} := b - Ax_{N-1}$ denotes the residual vector associated with the approximate solution x_{N-1} of (1.1). There are two reasons for the latter choice of \hat{v} . The vector $A^T r_{N-1}$ is parallel to the steepest descent direction for the functional

$$z \rightarrow \|Az - r_{N-1}\|^2,$$

and, therefore, we expect \hat{v} to give rapid decrease of the norm of the residual error. Moreover, $A^T r_{N-1}$ is the residual error for the normal equations associated with (1.1). It may be pertinent to evaluate the residual error for the normal equations regularly when the linear system of equations (1.1) is inconsistent, because when this error is small, an acceptable approximate solution of (1.1) may have been found. The main disadvantage of this choice of \hat{v} is that it requires a matrix-vector product evaluation with A^T . We therefore also present numerical examples when \hat{v} is determined by orthogonalization of a random vector.

When we replace the last column of V_N by \hat{v} , i.e., $v_N := \hat{v}$, we create a new matrix U_1 and put the old v_N there. Specifically, we let v_N be the first column, denoted by u_1 , of the matrix U_1 , i.e., $U_1 = [u_1]$. Thus, analogously to (3.1), we obtain

$$Av_{N-1} = h_{1,N-1}v_1 + \dots + h_{N-1,N-1}v_{N-1} + h_{N,N-1}u_1.$$

We can now compute a generalized Arnoldi decomposition, where, for $k := N, N+1, N+2, \dots$, until the next breakdown occurs, we require the columns V_k to be orthonormal, as well as orthogonal to U_1 . Thus, we obtain, for $k := N, N+1, N+2, \dots$, until another breakdown occurs,

$$Av_k - V_k(V_k^T Av_k) - U_1(U_1^T Av_k) = f_k.$$

If a new near-breakdown occurs, say, if the entry $h_{k+1,k} = \|f_k\|$ of \hat{H}_k is tiny, then the vector v_k is appended to the matrix U_1 ; i.e., we define $U_2 := [U_1, v_k]$, and a new unit vector, denoted by \hat{v} , which is orthogonal to all the columns of V_{k-1} and U_2 , is generated. We replace the last column of V_k by \hat{v} , and the computations are continued in a similar fashion as after the first near-breakdown. The following algorithm implements this process. The right-hand side vector b of (1.1) is not required to be of unit length in the algorithm. The vector h_k denotes the last column of the upper Hessenberg matrix H_k in (1.2). Further, $\hat{H}_{k-1}(k, :)$ denotes the k th row of the matrix \hat{H}_{k-1} . The function $\text{cond}(\hat{H}_k)$ evaluates the condition number $\|\hat{H}_k\| \|\hat{H}_k^\dagger\|$ of the matrix \hat{H}_k . The condition number is defined to be infinite if \hat{H}_k is not of full rank.

ALGORITHM 1 (Breakdown-Free GMRES (BFGMRES)).

```

1  Input:  $A \in \mathbb{R}^{n \times n}$ ,  $b \in \mathbb{R}^n$  ( $b \neq 0$ );  $tol$  (threshold for breakdown)
2  Initialize:  $v_1 := b/\|b\|$ ;  $p := 0$ ;  $V_1 := [v_1]$ ;  $U_0 := []$ ;  $\hat{H}_0 := []$ ;  $G_0 := []$ ;
3  for  $k := 1, 2, \dots$  until convergence
4       $w := Av_k$ ;
5       $h_k := V_k^T w$ ;  $g_k := U_p^T w$ ;
6       $w := w - V_k h_k - U_p g_k$ ;
7       $h_{k+1,k} := \|w\|$ ;
8       $\hat{H}_k := \begin{bmatrix} \hat{H}_{k-1} & h_k \\ 0 & h_{k+1,k} \end{bmatrix}$ ;
9      if  $\text{cond}(\hat{H}_k) > 1/tol$  then
10          $U_{p+1} := [U_p, v_k]$ ;
```

```

11    $G_{k-1} := \begin{bmatrix} G_{k-1} \\ \hat{H}_{k-1}(k, :) \end{bmatrix}; \hat{H}_{k-1}(k, :) := 0;$ 
12   Let  $\hat{v}$  be a unit vector, such that  $V_{k-1}^T \hat{v} = 0$ ,  $U_{p+1}^T \hat{v} = 0$ ;
13   Replace the last column  $v_k$  of  $V_k$  by  $\hat{v}$ , i.e., let  $v_k := \hat{v}$ ;
14    $w := Av_k;$ 
15    $h_k := V_k^T w; g_k := U_{p+1}^T w;$ 
16    $w := w - V_k h_k - U_{p+1} g_k;$ 
17    $h_{k+1,k} := \|w\|;$ 
18    $\hat{H}_k := \begin{bmatrix} \hat{H}_{k-1} & h_k \\ 0 & h_{k+1,k} \end{bmatrix};$ 
19   if  $\text{cond}(\hat{H}_k) > 1/\text{tol}$  then goto line 12;
20    $p := p + 1;$ 
21   endif
22    $v_{k+1} := w/h_{k+1,k};$ 
23    $V_{k+1} := [V_k, v_{k+1}];$ 
24   if  $p > 0$  then  $G_k := [G_{k-1}, g_k]$  else  $G_k := G_{k-1}$  endif
25   Solve  $\min_{y \in \mathbb{R}^k} \left\| \begin{bmatrix} \hat{H}_k \\ G_k \end{bmatrix} y - \|b\|e_1 \right\|$  for  $y_k$ ;
26    $x_k := V_k y_k;$ 
27 endfor

```

The following remarks provide some detailed explanations of the algorithm:

- Lines 4–7 and 22 describe the generalized Arnoldi process for generating the vector v_{k+1} . We orthogonalize w against the columns of V_k and, when the matrix U_p is not empty, against the columns of U_p as well. Lines 5–6 describe classical Gram–Schmidt orthogonalization; however, our implementation employs the modified Gram–Schmidt procedure. When a hard near-breakdown is detected in line 9, v_k , the last column of V_k , is appended to the matrix U_p to yield U_{p+1} . The matrices \hat{H}_{k-1} and G_{k-1} are updated in line 11 to yield the generalized Arnoldi decomposition

$$AV_{k-1} = V_k \hat{H}_{k-1} + U_{p+1} G_{k-1}.$$

A new vector \hat{v} , which replaces the column v_k of V_k , is generated in line 12. After one step of the generalized Arnoldi process (lines 14–18), we check in line 19 whether the vector \hat{v} yields a hard near-breakdown, in which case it is replaced. Otherwise, lines 22–24 yield the generalized Arnoldi decomposition

$$AV_k = V_{k+1} \tilde{H}_k + U_p G_k = [V_{k+1}, U_p] \tilde{H}_k,$$

where

$$\tilde{H}_k := \begin{bmatrix} \hat{H}_k \\ G_k \end{bmatrix}.$$

It is clear that the matrix $[V_{k+1}, U_p]$ has orthogonal columns.

- Lines 25–26 determine a solution that minimizes the residual error from $\mathcal{R}(V_k)$, analogously as in standard GMRES. Writing $x = V_k y$, we have

$$\begin{aligned} \|Ax - b\| &= \|[V_{k+1}, U_p] \tilde{H}_k y - \beta_0 [V_{k+1}, U_p] e_1\| \\ &= \|\tilde{H}_k y - \beta_0 e_1\|, \end{aligned}$$

where $\beta_0 := \|b\|$. Thus,

$$\min_{x \in \mathcal{R}(V_k)} \|Ax - b\| = \min_{y \in \mathbb{R}^k} \|\hat{H}_k y - \beta_0 e_1\|.$$

- Line 9 shows a simple criterion for a hard near-breakdown. We consider having reached a hard near-breakdown when the condition number $\text{cond}(\hat{H}_k)$ is larger than the threshold $1/\text{tol}$. Since \hat{H}_{k-1} is a submatrix of \hat{H}_k , the condition number is an increasing function of k . This criterion works well when $\text{cond}(\hat{H}_k)$ increases slowly for small values of k and then for some larger values of k increases rapidly. However, it is not always suitable when the condition number increases steadily to a large value as k increases, because then when $\text{cond}(\hat{H}_k) > 1/\text{tol}$, also $\text{cond}(\hat{H}_j) \approx 1/\text{tol}$ for $j \approx k$, and this can result in several consecutive near-breakdowns. To avoid this undesirable situation, we propose to reduce tol by a factor, say, 10^{-2} , when a near-breakdown is encountered; i.e., we replace line 9 by

$$(3.2) \quad \text{if } \text{cond}(\hat{H}_k) > 10^{2p}/\text{tol} \text{ then,}$$

where p is the number of hard near-breakdowns encountered so far during the computations. A further modification of line 9 is discussed below.

- What we have presented is a version of full GMRES in which the memory and computational cost increase quickly with the iteration. In practice, a restarted version, where the algorithm is restarted after a certain number of iterations, should be used.

Algorithm 1 searches for a solution outside the Krylov subspace K_{N-1} by introducing a new vector \hat{v} when a hard near-breakdown is detected. For singular matrices A with a null space of small dimension, hard near-breakdowns often do not occur until $N \approx n$ steps of the generalized Arnoldi process have been carried out. However, the component of the solution x of (1.1) in the Krylov subspace \mathcal{K}_{N-1} (i.e., \hat{x} in Theorem 2.1) sometimes can be approximated well by a vector x_k in a Krylov subspace \mathcal{K}_k of dimension $k \ll N - 1$, and then it would be desirable to introduce the new vector \hat{v} already after k steps of the generalized Arnoldi process. This situation may be difficult to detect, because the residual vector $r_k := b - Ax_k$ associated with x_k might not be of small norm. We have found that it can be advantageous to generate a new vector \hat{v} when the iterates x_k converge very slowly. This can be achieved by replacing line 9 of Algorithm 1 by

$$(3.3) \quad \text{if } (\text{cond}(\hat{H}_k) > 10^{2p}/\text{tol}) \text{ or } (\|x_k - x_{k-1}\| \leq \eta \|x_k\|) \text{ then,}$$

where η is a small positive constant of the order of the stopping tolerance and p is the number of hard near-breakdowns encountered during the computations so far; cf. (3.2).

We conclude this section with some comments on RRGMRRES. The k th iterate, x_k , determined by RRGMRRES, satisfies

$$\|b - Ax_k\| = \min_{z \in A\mathcal{K}_k} \|b - Az\|, \quad x_k \in A\mathcal{K}_k.$$

Thus, the iterate belongs to the range of A . Computed examples in [6] illustrate that RRGMRRES sometimes can yield computed solutions of higher quality than GMRES. We are therefore interested in an algorithm for BFRRGMRRES, a breakdown-free

variant of RRGMRRES. Such an algorithm can be obtained by a very minor modification of Algorithm 1: The initialization $v_1 := b/\|b\|$ in line 2 should be replaced by $v_1 := Ab/\|Ab\|$ and the vector $\|b\|e_1$ in line 25 has to be replaced by $[V_{k+1}, U_p]^T b$.

The following theorem discusses the behavior of RRGMRRES. We remark that the formulation of Theorem 3.3 in [5], which discusses related results, is incomplete. This has recently been pointed out by Cao and Wang [8].

THEOREM 3.1. *Let the matrix $A \in \mathbb{R}^{n \times n}$ be of rank $N < n$ and apply RRGMRRES with initial approximate solution $x_0 := 0$ to the solution of (1.1). Assume that RRGMRRES breaks down at step N . If $\dim(A^2\mathcal{K}_N) = N$, then RRGMRRES determines a least-squares solution of (1.1). If, instead, $\dim(A^2\mathcal{K}_N) < N$, then (1.1) has a solution in $A\mathcal{K}_N + \mathcal{R}(A^T)$.*

Proof. Assume that $\dim(A^2\mathcal{K}_N) = N$. This case is discussed by Cao and Wang [8]. Our proof is similar to the proof of Theorem 2.3 of section 2 and we use the same notation.

The Arnoldi process applied by RRGMRRES breaks down at step N and yields the decomposition

$$(3.4) \quad AV_N = V_N H_N, \quad V_N e_1 = Ab/\|Ab\|.$$

It follows from (3.4) and $\dim(A^2\mathcal{K}_N) = N$ that the matrix AV_N is of full rank and, therefore, that H_N is nonsingular. Moreover, $\mathcal{R}(V_N) \subset \mathcal{R}(A)$, and since $\text{rank}(V_N) = \text{rank}(A)$, it follows that $\mathcal{R}(V_N) = \mathcal{R}(A)$. The vector $\hat{x} \in \mathbb{R}^n$ is a least-squares solution of (1.1) if and only if the associated residual error is orthogonal to $\mathcal{R}(A)$, i.e., if and only if

$$(3.5) \quad 0 = V_N^T(A\hat{x} - b).$$

The linear system of equations

$$(3.6) \quad H_N y = V_N^T b$$

has a unique solution \hat{y} . It follows from (3.4) that $\hat{x} := V_N \hat{y}$ satisfies (3.5). Thus, \hat{x} is a least-squares solution of (1.1). RRGMRRES determines this solution. This is a benign breakdown.

We turn to the case when $\dim(A^2\mathcal{K}_N) < N$. It follows from this inequality and (3.4) that the upper Hessenberg H_N is singular. Similarly as above, $\mathcal{R}(V_N) = \mathcal{R}(A)$ and, therefore, $\hat{x} \in \mathbb{R}^n$ is a least-squares solution of (1.1) if and only if \hat{x} satisfies (3.5). However, differently from the situation above, the system of equations (3.6) might not have a solution, since H_N is singular. We circumvent this problem by appending a column to H_N as follows. Since H_N has positive subdiagonal entries, $\text{rank}(H_N) = N - 1$. Let $u \in \mathcal{N}(H_N^T)$ be of unit length and define $v := A^+ V_N u \in \mathcal{R}(A^T)$. It follows from $\mathcal{R}(V_N) = \mathcal{R}(A)$ that $Av = V_N u$ and, therefore, $V_N^T Av = u$. We seek a least-squares solution of the form

$$(3.7) \quad x = V_N y + v\eta, \quad y \in \mathbb{R}^N, \quad \eta \in \mathbb{R}.$$

Substituting this expression into (3.5) yields

$$(3.8) \quad 0 = V_N^T(AV_N y + Av\eta - b) = H_N y + u\eta - V_N^T b = [H_N, u] \begin{bmatrix} y \\ \eta \end{bmatrix} - e_1.$$

Since the matrix $[H_N, u] \in \mathbb{R}^{N \times (N+1)}$ is of full rank, (3.8) has a solution $\{\hat{y}, \hat{\eta}\}$. Substituting $y := \hat{y}$ and $\eta := \hat{\eta}$ into (3.7) yields a least-squares solution of (1.1). \square

Theorem 3.1 implies that RRGMRRES can be applied to solve inconsistent linear least-squares problems of the form (2.21).

4. Numerical examples. This section presents a few computed examples. All computations were carried out on an HP UNIX workstation using MATLAB with about 15 significant decimal digits. The initial approximate solution in all examples is chosen to be $x_0 := 0$.

Example 4.1. Consider a rectangular matrix of the form

$$(4.1) \quad \tilde{A} = \begin{bmatrix} \tilde{A}_{11} & 0 \\ \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix} \in \mathbb{R}^{n \times \ell},$$

where $\tilde{A}_{11} \in \mathbb{R}^{(n-k) \times (\ell-k)}$ is the sum of a random lower triangular matrix and $10I$, and $\tilde{A}_{21} \in \mathbb{R}^{k \times (\ell-k)}$ and $\tilde{A}_{22} \in \mathbb{R}^{k \times k}$ are random matrices generated by the MATLAB function `rand`.

We use GMRES and BFGMRES to solve the column-padded linear system of equations

$$(4.2) \quad Ax = b, \quad A := [\tilde{A}, 0] \in \mathbb{R}^{n \times n}, \quad x := \begin{bmatrix} \tilde{x} \\ 0 \end{bmatrix} \in \mathbb{R}^n,$$

where \tilde{A} is defined by (4.1). It is easy to see that if \tilde{A}_{22} is nonsingular and $n - \ell \geq k$, then A has k zero eigenvalues associated with Jordan blocks of size at least 2. We also apply the conjugate gradient method, using the CGLS implementation, to solve the normal equations,

$$(4.3) \quad A^T Ax = A^T b,$$

associated with (1.1).

For ease of notation we use the matrix A in (4.2) instead of \tilde{A} . Let $x_k \in \mathbb{R}^n$ denote the k th iterate determined by any one of the iterative methods considered. For consistent linear systems of equations (1.1), we plot the norm of the residual vectors,

$$(4.4) \quad r_k := b - Ax_k,$$

relative to the norm of r_0 for increasing values of k . When the linear system (1.1) is inconsistent, we instead plot the norm of the residual error associated with the normal equations (4.3),

$$(4.5) \quad \hat{r}_k := A^T b - A^T Ax_k,$$

relative to the norm of $A^T \hat{r}_0$, because $\|\hat{r}_k\|$ vanishes when x_k is a least-squares solution of (1.1), while $\|r_k\|$ does not.

We first consider a consistent linear system of equations (1.1) with A defined by (4.1) and $n := 1000$, $\ell := 700$, $k := 3$. Let the solution $\tilde{x} \in \mathbb{R}^\ell$ be a vector with random entries and define the right-hand side by $b := \tilde{A}\tilde{x}$.

We use the criterion (3.2) with $tol := 10^{-8}$ for detecting hard near-breakdowns in BFGMRES. The vector \hat{v} chosen in line 12 of Algorithm 1 at every hard near-breakdown is determined by orthogonalizing a random vector against the columns of the available matrices V_{k-1} and U_{p+1} . Here and throughout, the iterations are terminated when the relative residual $\|r_k\|/\|r_0\|$ drops below 10^{-14} (or $\|\hat{r}_k\|/\|\hat{r}_0\| < 10^{-14}$ for inconsistent systems).

The left-hand side graphs of Figure 4.1 show BFGMRES (solid curve) to reduce the norm of the residual error (4.4) faster than GMRES (dashed curve). We mark the

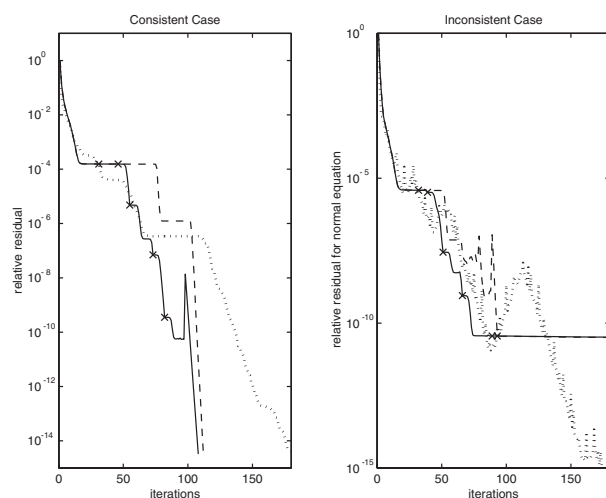


FIG. 4.1. Example 4.1: Convergence histories for overdetermined linear system for BFGMRES (solid curves with near-breakdowns marked by x), GMRES (dashed curves), and CGLS (dotted curves).

BFGMRES convergence curve by “x” where hard near-breakdowns occur. Here as well as in later examples, we see that there is typically significant reduction of the residual error a few iterations after a new vector is introduced. The nonmonotonic decrease of the norm of the residual error for BFGMRES near convergence is due to large round-off errors incurred when solving the reduced least-squares problem in line 25 of the algorithm. (Note that $\text{cond}(\hat{H}_k)$ steadily increases and may become very large at that stage of iterations.) We also display the norm of the residual errors associated with iterates determined by CGLS (dotted curve). The latter method is seen to require more iterations than BFGMRES and GMRES to reduce the relative residual to 10^{-14} , but CGLS is implemented without reorthogonalization, and therefore requires less memory and fewer vector operations per iteration. On the other hand, note that CGLS needs the evaluation of two matrix-vector products in each iteration, one with A and one with A^T , while each iteration of BFGMRES or GMRES requires only the evaluation of one matrix-vector product with A .

We next illustrate the performance of BFGMRES, GMRES, and CGLS when applied to the solution of an inconsistent overdetermined linear system of equations. Such a system of equations is obtained by perturbing the right-hand side in (4.2). Specifically, we generate the right-hand side with the Matlab instruction $\mathbf{b} = \mathbf{A} * \mathbf{x} + 1\mathbf{e}-6 * \mathbf{rand}(\mathbf{n}, 1)$, where $\mathbf{x}^T := [\tilde{x}^T, 0^T]$ and $\tilde{x} \in \mathbb{R}^\ell$ is the same random vector as above. The right-hand side graphs of Figure 4.1 show the norm of the residual errors (4.5) for the iterates x_k determined by GMRES, BFGMRES, and CGLS. GMRES and BFGMRES reduce the norm of the residual (4.5) by about a factor 10^{-11} , but thereafter the norm of the residual does not decrease further. BFGMRES converges somewhat faster than GMRES and gives a smoother reduction of the norm of the residual error. CGLS converges slower but is able to reduce the norm of the residual (4.5) by a factor 10^{-14} .

We turn to an underdetermined linear system of equations, obtained by using the transpose of the matrix A employed in the computations above. Thus, we would like

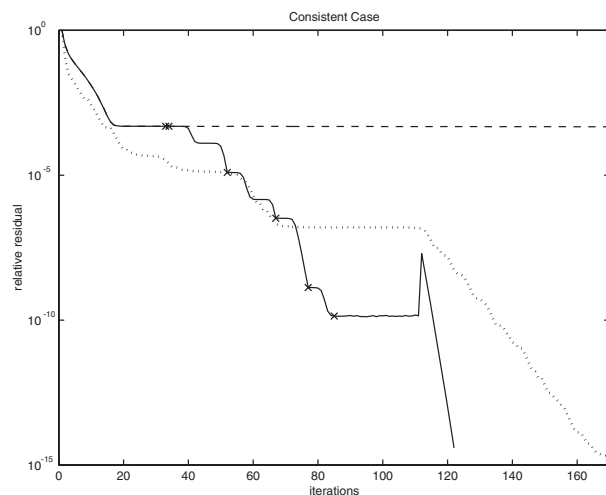


FIG. 4.2. Example 4.1: Convergence histories for underdetermined linear system for BFGMRES (solid curve with near-breakdowns marked by x), GMRES (dashed curve), and CGLS (dotted curve).

to solve

$$\tilde{A}^T y = \tilde{c},$$

where $y \in \mathbb{R}^n$ is a random vector and the right-hand side is defined by $\tilde{c} := \tilde{A}^T y$. BFGMRES and GMRES are applied to the associated row-padded system

$$(4.6) \quad A^T y = \begin{bmatrix} \tilde{c} \\ 0 \end{bmatrix}.$$

Figure 4.2 displays the norm of the residual error (4.4) for iterates computed by BFGMRES (solid curve), GMRES (dashed curve), and CGLS (dotted curve). Due to the structure of the linear system of equations (4.6), the last $n - m$ components of all vectors v_i determined by GMRES vanish. Therefore, GMRES cannot reduce the norm of the relative residual error below $5 \cdot 10^{-4}$. On the other hand, BFGMRES expands the subspace in which the computed solution is being sought, and the computed iterates converge to a solution of the linear system. Figure 4.2 shows BFGMRES to reduce the norm of the residual error (4.4) faster than any of the other methods considered.

Finally, we illustrate the finite termination property of Theorem 2.7 by solving an inconsistent overdetermined linear system of equations of the same form, but of smaller size, than the overdetermined system considered above. Thus, we solve an inconsistent system (4.2) with A of the form (4.1) with $n := 100$, $\ell := 70$, $k := 1$. The diagonal elements of A_{11} are $1, 2, \dots, 69$. We compare the three methods both with and without reorthogonalization (for CGLS the residual vectors of the normal equations (4.5) are reorthogonalized). The graphs on the left-hand side of Figure 4.3 show the norm of the residual error for the normal equations converge for all three methods when reorthogonalization is carried out. The graphs show the relative residual norm to drop to 10^{-15} at step 71 (which is $N+1$) for GMRES and BFGMRES, but at step 70 for CGLS. This is consistent with the theory (Theorem 2.7). The graphs on the right-hand side of Figure 4.3 show the performance of the methods when no

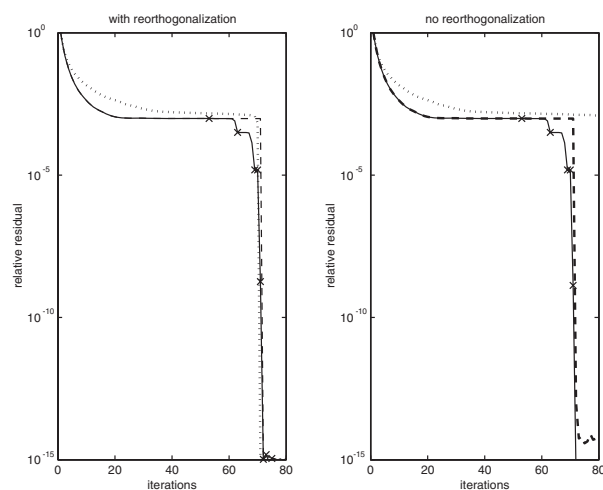


FIG. 4.3. *Example 4.1: Convergence histories for overdetermined linear system for BFGMRES (solid curves with near-breakdowns marked by x), GMRES (dashed curves), and CGLS (dotted curves).*

reorthogonalization has been carried out. GMRES and BFGMRES can be seen to behave similarly as with reorthogonalization, while iterates determined by CGLS do not appear to converge.

The next two examples are taken from Brown and Walker [4].

Example 4.2. Consider the nonsymmetric tridiagonal matrix

$$(4.7) \quad A := \begin{bmatrix} 0 & 1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & -1 & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

For odd values of n , A is singular with index one. In particular, $\mathcal{N}(A) = \mathcal{N}(A^T)$. Let $n := 49$ and $b := [1, 0, \dots, 0, 1]^T$ as in [4]. This yields an inconsistent linear system of equations (1.1). GMRES applied to this system computes a sequence of approximate solutions. At step 24 a hard near-breakdown is detected. Nevertheless, GMRES is able to determine a least-squares solution of the linear system of equations. The criterion used for detecting a near-breakdown is the same as in Example 4.1.

Now replace the right-hand side vector by $b := [1, 0, \dots, 0, 1 + 10^{-10}]^T$. GMRES applied to (1.1) with this new right-hand side vector decreases the norm of the residual error of the associated normal equations (4.5) to 10^{-10} at step 24. However, in the next step the norm of the residual error increases by about a factor 10^4 due to high sensitivity to round-off errors. The residual error stays at this level for the next 25 iterations until it quickly drops to 10^{-14} . Figure 4.4 displays the convergence histories of the residual errors (4.5) for BFGMRES (solid curve) and GMRES (dashed curve). We see that BFGMRES yields a smoother decrease of the residual error than GMRES. The plateau in convergence of BFGMRES after step 24 appears to be due to the matrix itself as different choices of \hat{v} result in similar convergence curves.

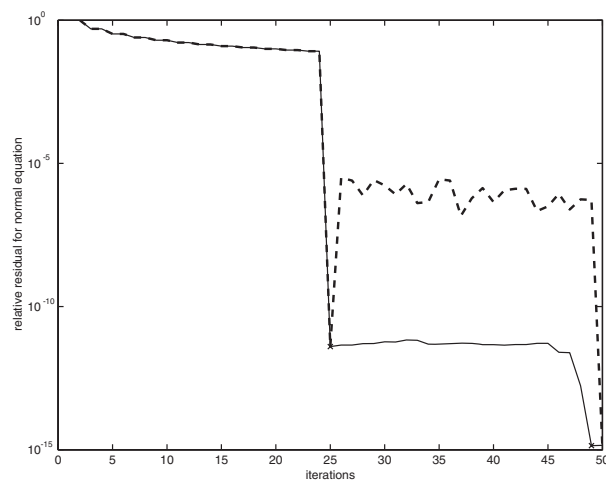


FIG. 4.4. *Example 4.2: Convergence histories for BFGMRES (solid curve with near-breakdowns marked by x) and GMRES (dashed curve).*

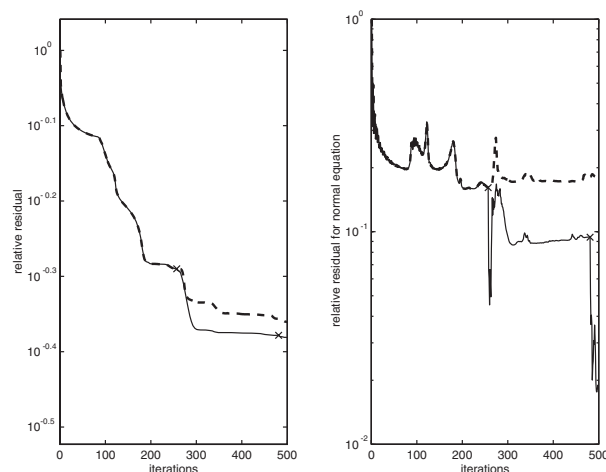


FIG. 4.5. *Example 4.3: Convergence histories for BFGMRES (solid curves with near-breakdowns marked by x) and GMRES (dashed curves).*

Example 4.3. We discretize the partial differential equation

$$\Delta u + d \frac{\partial u}{\partial z_1} = f, \quad z := [z_1, z_2] \in [0, 1]^2,$$

with Neumann boundary condition using centered finite differences on an $m \times m$ regular mesh; see [4, Experiment 4.3] for a description of the matrix so obtained. We used $m := 63$, $d := 10$, and

$$f(z) := z_1 + z_2 + \sin(10z_1) \cos(10z_2) + \exp(10z_1 z_2).$$

This yields an inconsistent linear system of equations which is fairly difficult to solve;

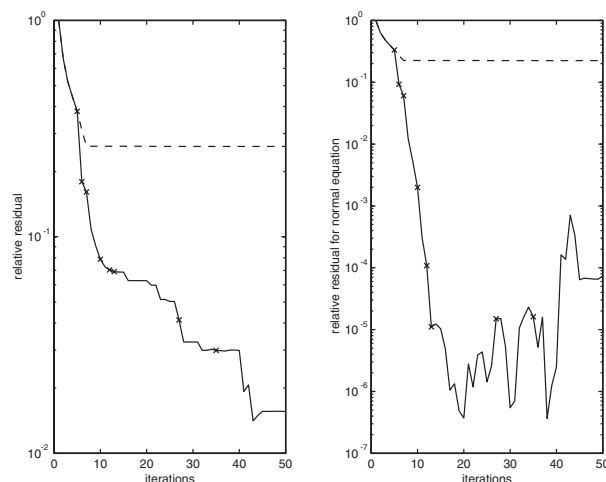


FIG. 4.6. Example 4.4: Convergence histories for BFRGMRES (solid curves with near-breakdowns marked by \times) and RRGMRMRES (dashed curves).

in particular, $\mathcal{N}(A^T) \neq \mathcal{N}(A)$. We use the criterion (3.3) with $\text{tol} := 10^{-8}$ and $\eta := 10^{-6}$. The vector \hat{v} chosen in line 12 of Algorithm 1 at every hard near-breakdown is determined by orthogonalizing $A^T r_k$ against the columns of the available matrices V_{k-1} and U_{p+1} , where r_k denotes the residual vector (4.4) associated with the present iterate.

The convergence histories for GMRES and BFGMRMRES are shown in Figure 4.5. The condition numbers of the matrices \hat{H}_k determined by GMRES increase steadily to about 10^{15} as k increases, while the condition numbers of the analogous matrices computed by BFGMRMRES are bounded by about 10^9 . The smaller condition numbers associated with BFGMRMRES may help this method to achieve better convergence than GMRES.

Example 4.4. Our last example is generated by the Matlab function `parallax` in Regularization Tools by Hansen [13]. We used `parallax` to determine a rank-deficient matrix $\tilde{A} \in \mathbb{R}^{26 \times 5000}$ and an associated right-hand side vector $b \in \mathbb{R}^{26}$. According to the Matlab function `rank`, the matrix \tilde{A} has rank 24.

We apply RRGMRMRES and BFRGMRES with full reorthogonalization to solve the underdetermined least-squares problem after row-padding of \tilde{A} . The graphs in the left-hand side of Figure 4.6 show the convergence histories of the norm of residual errors (4.4), and the graphs in the right-hand side of the figure display the convergence histories of the norm of residual errors of the normal equations (4.5) for BFRGMRES (solid curves) and RRGMRMRES (dotted curves). The curves for BFRGMRES vary less erratically than the curves for RRGMRMRES. Moreover, BFRGMRES reduces the residual errors to a smaller value than RRGMRMRES.

In summary, our numerical examples demonstrate BFGMRMRES and BFRGMRES to have more desirable convergence behavior than GMRES and RRGMRMRES, respectively, when applied to the solution of singular systems.

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