CG VERSUS MINRES: AN EMPIRICAL COMPARISON*

DAVID CHIN-LUNG FONG† AND MICHAEL SAUNDERS‡

Abstract. For iterative solution of symmetric systems $Ax = b$, the conjugate gradient method (CG) is commonly used when A is positive definite, while the minimum residual method (MINRES) is typically reserved for indefinite systems. We investigate the sequence of approximate solutions x_k generated by each method and suggest that even if A is positive definite, MINRES may be preferable to CG if iterations are to be terminated early. In particular, we show for MINRES that the solution norms $\|x_k\|$ are monotonically increasing when A is positive definite (as was already known for CG), and the solution errors $\|x^* - x_k\|$ are monotonically decreasing. We also show that the backward errors for the MINRES iterates x_k are monotonically decreasing.

Key words. conjugate gradient method, minimum residual method, iterative method, sparse matrix, linear equations, CG, CR, MINRES, Krylov subspace method, trust-region method

1. Introduction. The conjugate gradient method (CG) [11] and the minimum residual method (MINRES) [18] are both Krylov subspace methods for the iterative solution of symmetric linear equations $Ax = b$. CG is commonly used when the matrix A is positive definite, while MINRES is generally reserved for indefinite systems [27, p85]. We reexamine this wisdom from the point of view of early termination on positive-definite systems.

We assume that the system $Ax = b$ is real with A symmetric positive definite (spd) and of dimension $n \times n$. The Lanczos process [13] with starting vector b may be used to generate the $n \times k$ matrix $V_k \equiv \begin{pmatrix} v_1 & v_2 & \dots & v_k \end{pmatrix}$ and the $(k+1) \times k$ Hessenberg tridiagonal matrix $\underline{T_k}$ such that $AV_k = V_{k+1}\underline{T_k}$ for $k = 1, 2, \dots, \ell$ and $AV_\ell = V_\ell T_\ell$ for some $\ell \le n$, where the columns of V_k form a theoretically orthonormal basis for the kth Krylov subspace $\mathcal{K}_k(A, b) \equiv \text{span}\{b, Ab, A^2b, \dots, A^{k-1}b\}$, and T_ℓ is $\ell \times \ell$ and tridiagonal. Approximate solutions within the kth Krylov subspace may be formed as $x_k = V_k y_k$ for some k-vector y_k. As shown in [18], three iterative methods CG, MINRES, and SYMMLQ may be derived by choosing y_k appropriately at each iteration. CG is well defined if A is spd, while MINRES and SYMMLQ are stable for any symmetric nonsingular A.

As noted by Choi [2], SYMMLQ can form an approximation $x_{k+1} = V_{k+1}y_{k+1}$ in the $(k+1)$th Krylov subspace when CG and MINRES are forming their approximations $x_k = V_k y_k$ in the kth subspace. It would be of future interest to compare all three methods on spd systems, but for the remainder of this paper we focus on CG and MINRES.

With different methods using the same information V_{k+1} and $\underline{T_k}$ to compute solution estimates $x_k = V_k y_k$ within the same Krylov subspace (for each k), it is commonly thought that the number of iterations required will be similar for each method, and hence CG should be preferable on spd systems because it requires somewhat fewer floating-point operations per iteration. This view is justified if an accurate solution is required (stopping tolerance τ close to machine precision ϵ). We show that with

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looser stopping tolerances, MINRES is sure to terminate sooner than CG when the stopping rule is based on the backward error for x_k, and by numerical examples we illustrate that the difference in iteration numbers can be substantial.

1.1. Notation. We study the application of CG and MINRES to real symmetric positive-definite (spd) systems $Ax = b$. The unique solution is denoted by x^*. The initial approximate solution is $x_0 \equiv 0$, and $r_k \equiv b - Ax_k$ is the residual vector for an approximation x_k within the kth Krylov subspace. For a vector v and matrix A, $\|v\|$ and $\|A\|$ denote the 2-norm and the Frobenius norm respectively, and $A \succ 0$ indicates that A is spd.

2. Minimization properties of Krylov subspace methods. With exact arithmetic, the Lanczos process terminates with $k = \ell$ for some $\ell \leq n$. To ensure that the approximations $x_k = V_k y_k$ improve by some measure as k increases toward ℓ, the Krylov solvers minimize some convex function within the expanding Krylov subspaces [9].

2.1. CG. When A is spd, the quadratic form $\phi(x) \equiv \frac{1}{2}x^T Ax - b^T x$ is bounded below, and its unique minimizer solves $Ax = b$. A characterization of the CG iterations is that they minimize the quadratic form within each Krylov subspace [9], [17, §2.4], [28, §§8.8–8.9]:

$$x_k^C = V_k y_k^C, \quad \text{where} \quad y_k^C = \arg\min_y \phi(V_k y).$$

With $b = Ax^*$ and $2\phi(x_k) = x_k^T Ax_k - 2x_k^T Ax^*$, this is equivalent to minimizing the function $\|x^* - x_k\|_A \equiv (x^* - x_k)^T A(x^* - x_k)$, known as the *energy norm of the error*, within each Krylov subspace. For some applications, this is a desirable property [21, 24, 1, 17, 28].

2.2. MINRES. For nonsingular (and possibly indefinite) systems, the residual norm was used in [18] to characterize the MINRES iterations:

$$x_k^M = V_k y_k^M, \quad \text{where} \quad y_k^M = \arg\min_y \|b - AV_k y\|. \tag{2.1}$$

Thus, MINRES minimizes $\|r_k\|$ within the kth Krylov subspace. This was also an aim of Stiefel's Conjugate Residual method (CR) [23] for spd systems (and of Luenberger's extensions of CR to indefinite systems [15, 16]). Thus, CR and MINRES must generate the same iterates on spd systems. We use this connection to prove that $\|x_k\|$ increases monotonically when MINRES is applied to an spd system.

2.3. CG and CR. The two methods for solving spd systems $Ax = b$ are summarized in Table 2.1. The first two columns are pseudocodes for CG and CR with iteration number k omitted for clarity; they match our MATLAB implementations. Note that $q = Ap$ in both methods, but it is not computed as such in CR. Termination occurs when $r = 0$ ($\Rightarrow \rho = \beta = 0$).

To prove our main result we need to introduce iteration indices; see column 3 of Table 2.1. Termination occurs when $r_k = 0$ for some index $k = \ell \leq n$ ($\Rightarrow \rho_\ell = \beta_\ell = 0$, $r_\ell = s_\ell = p_\ell = q_\ell = 0$). Note: This ℓ is the same as the ℓ at which the Lanczos process theoretically terminates for the given A and b.

THEOREM 2.1. *The following properties hold for Algorithm CR:*
(a) $q_i^T q_j = 0$ *(*$i \neq j$*)*
(b) $r_i^T q_j = 0$ *(*$i \geq j + 1$*)*

TABLE 2.1
Pseudocode for algorithms CG and CR

CG	CR	CR
Initialize	Initialize	Initialize
$x = 0$, $r = b$	$x = 0$, $r = b$, $s = Ar$,	$x_0 = 0$, $r_0 = b$, $s_0 = Ar_0$,
$\rho = \|r\|^2$, $p = r$	$\rho = r^T s$, $p = r$, $q = s$	$\rho_0 = r_0^T s_0$, $p_0 = r_0$, $q_0 = s_0$
Repeat	Repeat	For $k = 1, 2, \ldots$
$q = Ap$	$(q = Ap)$	$(q_{k-1} = Ap_{k-1})$
$\alpha = \rho / p^T q$	$\alpha = \rho / \|q\|^2$	$\alpha_k = \rho_{k-1} / \|q_{k-1}\|^2$
$x \leftarrow x + \alpha p$	$x \leftarrow x + \alpha p$	$x_k = x_{k-1} + \alpha_k p_{k-1}$
$r \leftarrow r - \alpha q$	$r \leftarrow r - \alpha q$	$r_k = r_{k-1} - \alpha_k q_{k-1}$
	$s = Ar$	$s_k = Ar_k$
$\bar{\rho} = \rho$, $\rho = r^T r$	$\bar{\rho} = \rho$, $\rho = r^T s$	$\rho_k = r_k^T s_k$
$\beta = \rho / \bar{\rho}$	$\beta = \rho / \bar{\rho}$	$\beta_k = \rho_k / \rho_{k-1}$
$p \leftarrow r + \beta p$	$p \leftarrow r + \beta p$	$p_k = r_k + \beta_k p_{k-1}$
	$q \leftarrow s + \beta q$	$q_k = s_k + \beta_k q_{k-1}$

Proof. Given in [16, Theorem 1]. □

THEOREM 2.2. *The following properties hold for Algorithm CR:*

(a) $\alpha_i \geq 0$
(b) $\beta_i \geq 0$
(c) $p_i^T q_j \geq 0$
(d) $p_i^T p_j \geq 0$
(e) $x_i^T p_j \geq 0$
(f) $r_i^T p_j \geq 0$

Proof.

(a) Here we use the fact that A is spd. The inequalities are strict until $i = \ell$ (and $r_\ell = 0$).

$$\begin{aligned} \rho_i &= r_i^T s_i = r_i^T A r_i \geq 0 \qquad (A \succ 0) \\ \alpha_i &= \rho_{i-1} / \|q_{i-1}\|^2 \geq 0 \end{aligned} \tag{2.2}$$

(b) And again:

$$\beta_i = \rho_i / \rho_{i-1} \geq 0 \qquad \text{(by (2.2))}$$

(c) Case I: $i = j$

$$p_i^T q_i = p_i^T A p_i \geq 0 \qquad (A \succ 0)$$

Case II: $i - j = k > 0$

$$\begin{aligned} p_i^T q_j = p_i^T q_{i-k} &= r_i^T q_{i-k} + \beta_i p_{i-1}^T q_{i-k} \\ &= \beta_i p_{i-1}^T q_{i-k} \qquad \text{(by Thm 2.1 (b))} \\ &\geq 0, \end{aligned}$$

where $\beta_i \geq 0$ by (b) and $p_{i-1}^T q_{i-k} \geq 0$ by induction as $(i-1)-(i-k) = k-1 < k$.

Case III: $j - i = k > 0$

$$\begin{aligned} p_i^T q_j = p_i^T q_{i+k} &= p_i^T A p_{i+k} \\ &= p_i^T A(r_{i+k} + \beta_{i+k} p_{i+k-1}) \\ &= q_i^T r_{i+k} + \beta_{i+k} p_i^T q_{i+k-1} \\ &= \beta_{i+k} p_i^T q_{i+k-1} && \text{(by Thm 2.1 (b))} \\ &\geq 0, \end{aligned}$$

where $\beta_{i+k} \geq 0$ by (b) and $p_i^T q_{i+k-1} \geq 0$ by induction as $(i+k-1)-i = k-1 < k$.

(d) At termination, define $\mathcal{P} \equiv \text{span}\{p_0, p_1, \ldots, p_{\ell-1}\}$ and $\mathcal{Q} \equiv \text{span}\{q_0, \ldots, q_{\ell-1}\}$. By construction, $\mathcal{P} = \text{span}\{b, Ab, \ldots, A^{\ell-1}b\}$ and $\mathcal{Q} = \text{span}\{Ab, \ldots, A^{\ell}b\}$ (since $q_i = Ap_i$). Again by construction, $x_\ell \in \mathcal{P}$, and since $r_\ell = 0$ we have $b = Ax_\ell \Rightarrow b \in \mathcal{Q}$. We see that $\mathcal{P} \subseteq \mathcal{Q}$. By Theorem 2.1(a), $\{q_i/\|q_i\|\}_{i=0}^{\ell-1}$ forms an orthonormal basis for $\mathcal{Q}$. If we project $p_i \in \mathcal{P} \subseteq \mathcal{Q}$ onto this basis, we have

$$p_i = \sum_{k=0}^{\ell-1} \frac{p_i^T q_k}{q_k^T q_k} q_k,$$

where all coordinates are non-negative from (c). Similarly for any other p_j, $j < \ell$. Therefore $p_i^T p_j \geq 0$ for any $i, j < \ell$.

(e) By construction,

$$x_i = x_{i-1} + \alpha_i p_{i-1} = \cdots = \sum_{k=1}^{i} \alpha_k p_{k-1} \qquad (x_0 = 0)$$

Therefore $x_i^T p_i \geq 0$ by (d) and (a).

(f) Note that any r_i can be expressed as a sum of q_i:

$$\begin{aligned} r_i &= r_{i+1} + \alpha_{i+1} q_i \\ &= \cdots \\ &= r_l + \alpha_l q_{l-1} + \cdots + \alpha_{i+1} q_i \\ &= \alpha_l q_{l-1} + \cdots + \alpha_{i+1} q_i. \end{aligned}$$

Thus we have

$$r_i^T p_j = (\alpha_l q_{l-1} + \cdots + \alpha_{i+1} q_i)^T p_j \geq 0,$$

where the inequality follows from (a) and (c).

□

We are now able to prove our main theorem about the monotonic increase of $\|x_k\|$ for CR and MINRES. A similar result was proved for CG by Steihaug [21].

THEOREM 2.3. *For CR (and hence MINRES) on an spd system $Ax = b$, $\|x_k\|$ increases monotonically.*

Proof. $\|x_i\|^2 - \|x_{i-1}\|^2 = 2\alpha_i x_{i-1}^T p_{i-1} + p_{i-1}^T p_{i-1} \geq 0$, where the last inequality follows from Theorem 2.2 (a), (d) and (e). Therefore $\|x_i\| \geq \|x_{i-1}\|$. □

$\|x^* - x_k\|$ is known to be monotonic for CG [11]. The corresponding result for CR is a direct consequence of [11, Thm 7:5]. However, the second half of that theorem,

$\|x^* - x_{k-1}^C\| > \|x^* - x_k^M\|$, rarely holds in machine arithmetic. We give here an alternative proof that does not depend on CG.

THEOREM 2.4. *For CR (and hence MINRES) on an spd system $Ax = b$, the error $\|x^* - x_k\|$ decreases monotonically.*

Proof. From the update rule for x_k, we can express the final solution $x_l = x^*$ as

$$\begin{aligned} x_l &= x_{l-1} + \alpha_{l-1} p_{l-1} \\ &= \cdots \\ &= x_k + \alpha_{k+1} p_k + \cdots + \alpha_{l-1} p_{l-1} && (2.3) \\ &= x_{k-1} + \alpha_k p_{k-1} + \alpha_{k+1} p_k + \cdots + \alpha_{l-1} p_{l-1}. && (2.4) \end{aligned}$$

Using the last two equalities above, we can write

$$\begin{aligned} \|x_l - x_{k-1}\|^2 - \|x_l - x_k\|^2 &= (x_l - x_{k-1})^T (x_l - x_{k-1}) - (x_l - x_k)^T (x_l - x_k) \\ &= 2\alpha_k p_{k-1}^T (\alpha_{k+1} p_k + \cdots + \alpha_{l-1} p_{l-1}) + \alpha_k^2 p_{k-1}^T p_{k-1} \\ &\geq 0, \end{aligned}$$

where the last inequality follows from Theorem 2.2 (a), (d). □

The energy norm error $\|x^* - x_k\|_A$ is monotonic for CG by design. The corresponding result for CR is given in [11, Thm 7:4]. We give an alternative proof here.

THEOREM 2.5. *For CR (and hence MINRES) on an spd system $Ax = b$, the error in energy norm $\|x^* - x_k\|_A$ is strictly decreasing.*

Proof. From (2.3) and (2.4), we can write

$$\begin{aligned} &\|x_l - x_{k-1}\|_A^2 - \|x_l - x_k\|_A^2 \\ &= (x_l - x_{k-1})^T A (x_l - x_{k-1}) - (x_l - x_k)^T A (x_l - x_k) \\ &= 2\alpha_k p_{k-1}^T A (\alpha_{k+1} p_k + \cdots + \alpha_{l-1} p_{l-1}) + \alpha_k^2 p_{k-1}^T A p_{k-1} \\ &= 2\alpha_k q_{k-1}^T (\alpha_{k+1} p_k + \cdots + \alpha_{l-1} p_{l-1}) + \alpha_k^2 q_{k-1}^T p_{k-1} \\ &> 0, \end{aligned}$$

where the last inequality follows from Theorem 2.2 (a), (c). □

3. Backward error analysis. For many physical problems requiring numerical solution, we are given inexact or uncertain input data (in this case A and/or b). It is not justifiable to seek a solution beyond the accuracy of the data [6]. Instead, it is more reasonable to stop an iterative solver once we know that the current approximate solution solves a *nearby problem*. The measure of "nearby" should match the error in the input data. The design of such stopping rules is an important application of *backward error analysis*.

For a consistent linear system $Ax = b$, we think of x_k coming from the kth iteration of one of the iterative solvers. Following Titley-Péloquin [25] we say that x_k is an *acceptable solution* if and only if there exist perturbations E and f satisfying

$$(A + E)x_k = b + f, \qquad \frac{\|E\|}{\|A\|} \leq \alpha, \qquad \frac{\|f\|}{\|b\|} \leq \beta \tag{3.1}$$

for some tolerances $\alpha \geq 0$, $\beta \geq 0$ that reflect the (preferably known) accuracy of the data. We are naturally interested in minimizing the size of E and f. If we define the optimization problem

$$\min_{\xi, E, f} \xi \ \text{ s.t. } \ (A + E)x_k = b + f, \quad \frac{\|E\|}{\|A\|} \leq \alpha\xi, \quad \frac{\|f\|}{\|b\|} \leq \beta\xi$$

to have optimal solution ξ_k, E_k, f_k (all functions of x_k, α, and β), we see that x_k is an acceptable solution if and only if $\xi_k \le 1$. We call ξ_k the *normwise relative backward error* (NRBE) for x_k.

With $r_k = b - Ax_k$, the optimal solution ξ_k, E_k, f_k is shown in [25] to be

$$\phi_k = \frac{\beta\|b\|}{\alpha\|A\|\|x_k\| + \beta\|b\|}, \qquad E_k = \frac{(1-\phi_k)}{\|x_k\|^2} r_k x_k^T, \tag{3.2}$$

$$\xi_k = \frac{\|r_k\|}{\alpha\|A\|\|x_k\| + \beta\|b\|}, \qquad f_k = -\phi_k r_k. \tag{3.3}$$

(See [12, p12] for the case $\beta = 0$ and [12, §7.1 and p336] for the case $\alpha = \beta$.)

3.1. Stopping rule. For general tolerances α and β, the condition $\xi_k \le 1$ for x_k to be an acceptable solution becomes

$$\|r_k\| \le \alpha\|A\|\|x_k\| + \beta\|b\|, \tag{3.4}$$

the stopping rule used in LSQR for consistent systems [19, p54, rule S1].

3.2. Monotonic backward errors. Of interest is the *size* of the perturbations to A and b for which x_k is an exact solution of $Ax = b$. From (3.2)–(3.3), the perturbations have the following norms:

$$\|E_k\| = (1-\phi_k)\frac{\|r_k\|}{\|x_k\|} = \frac{\alpha\|A\|\|r_k\|}{\alpha\|A\|\|x_k\| + \beta\|b\|}, \tag{3.5}$$

$$\|f_k\| = \phi_k\|r_k\| = \frac{\beta\|b\|\|r_k\|}{\alpha\|A\|\|x_k\| + \beta\|b\|}. \tag{3.6}$$

Since $\|x_k\|$ is monotonically increasing for CG and MINRES, we see from (3.2) that ϕ_k is monotonically decreasing for both solvers. Since $\|r_k\|$ is monotonically decreasing for MINRES (but not for CG), we have the following result.

THEOREM 3.1. *Suppose $\alpha > 0$ and $\beta > 0$ in* (3.1). *For CR and MINRES (but not CG), the relative backward errors $\|E_k\|/\|A\|$ and $\|f_k\|/\|b\|$ decrease monotonically.*

Proof. This follows from (3.5)–(3.6) with $\|x_k\|$ increasing for both solvers and $\|r_k\|$ decreasing for CR and MINRES but not for CG. □

4. Numerical results. Here we compare the convergence of CG and MINRES on various spd systems $Ax = b$ and some associated indefinite systems $(A - \delta I)x = b$. The test examples are drawn from the University of Florida Sparse Matrix Collection (Davis [5]). We experimented with all 26 cases for which A is real spd and b is supplied. In MATLAB we computed the condition number for each test matrix by finding the largest and smallest eigenvalue using `eigs(A,1,'LM')` and `eigs(A,1,'SM')` respectively. For this test set, the condition numbers range from 1.7E+03 to 3.1E+13.

Since A is spd, we apply diagonal preconditioning by redefining A and b as follows: $d = \mathrm{diag}(A)$, $D = \mathrm{diag}(1./\mathrm{sqrt}(d))$, $A \leftarrow DAD$, $b \leftarrow Db$, $b \leftarrow b/\|b\|$. Thus in the figures below we have $\mathrm{diag}(A) = I$ and $\|b\| = 1$. With this preconditioning, the condition numbers range from 1.2E+01 to 2.2E+11. The distribution of condition number of the test set matrices before and after preconditioning is shown in Figure 4.1.

The stopping rule used for CG and MINRES was (3.4) with $\alpha = 0$ and $\beta = 10^{-8}$. That is, $\|r_k\| \le 10^{-8}\|b\| = 10^{-8}$ (but with a maximum of $5n$ iterations for spd systems and n iterations for indefinite systems).

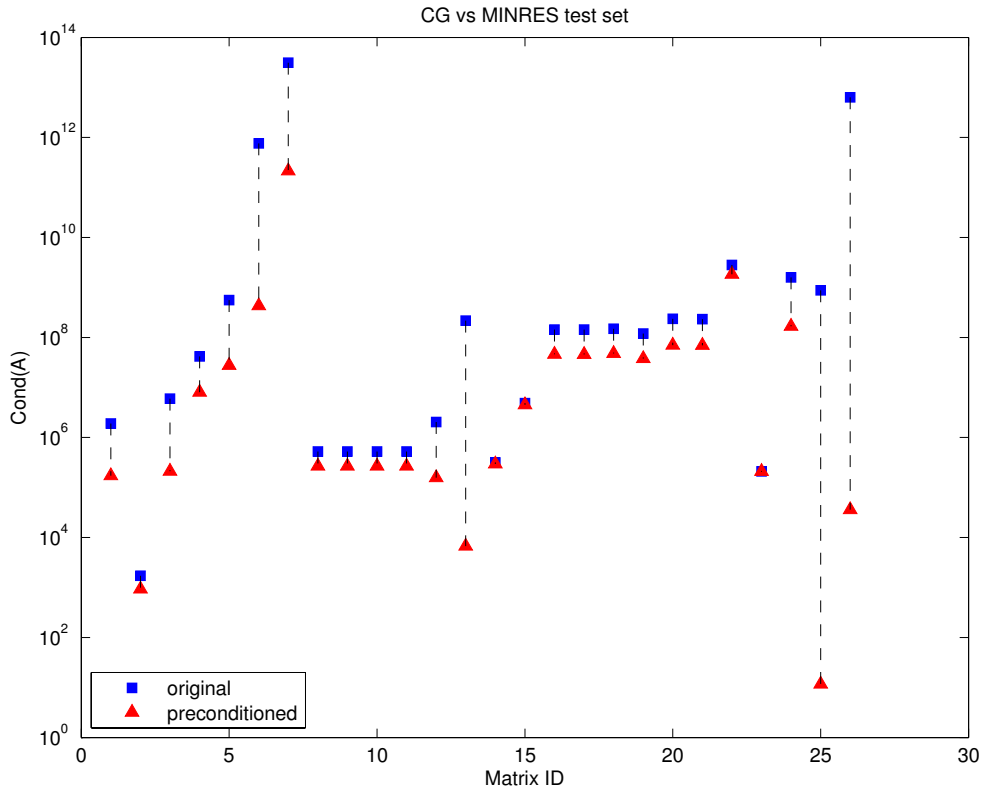

FIG. 4.1. *Distribution of condition number for matrices used for CG vs MINRES comparison, before and after diagonal preconditioning*

4.1. Positive-definite systems. In plotting backward errors, we assume for simplicity that $\alpha > 0$ and $\beta = 0$ in (3.1)–(3.3), even though it doesn't match the choice of α and β in the stopping rule (3.4). This gives $\phi_k = 0$ and $\|E_k\| = \|r_k\|/\|x_k\|$ in (3.5). Thus, as in Theorem 3.1, we expect $\|E_k\|$ to decrease monotonically for CR and MINRES but not for CG.

In Figures 4.2 and 4.3, we plot $\|r_k\|/\|x_k\|$, $\|x^* - x_k\|_A$, and $\|x^* - x_k\|$ for CG and MINRES for four different problems. For CG, the plots confirm that $\|x^* - x_k\|_A$ and $\|x^* - x_k\|$ are monotonic. For MINRES, the plots confirm the prediction of Theorems 3.1, 2.5, and 2.4 that $\|r_k\|/\|x_k\|$, $\|x^* - x_k\|_A$, and $\|x^* - x_k\|$ are monotonic.

Figure 4.2 (left) shows problem `Schenk_AFE_af_shell8` with A of size 504855×504855 and $\text{cond}(A) = 2.7\text{E}{+}05$. From the plot of backward errors $\|r_k\|/\|x_k\|$, we see that both CG and MINRES converge quickly at the early iterations. Then the backward error of MINRES plateaus at about iteration 80, and the backward error of CG stays about 1 order of magnitude behind MINRES. A similar phenomenon of fast convergence at early iterations followed by slow convergence is observed in the energy norm error and 2-norm error plots.

Figure 4.2 (right) shows problem `Cannizzo_sts4098` with A of size 4098×4098 and $\text{cond}(A) = 6.7\text{E}{+}03$. MINRES converges slightly faster in terms of backward error, while CG converges slightly faster in terms of both error norms.

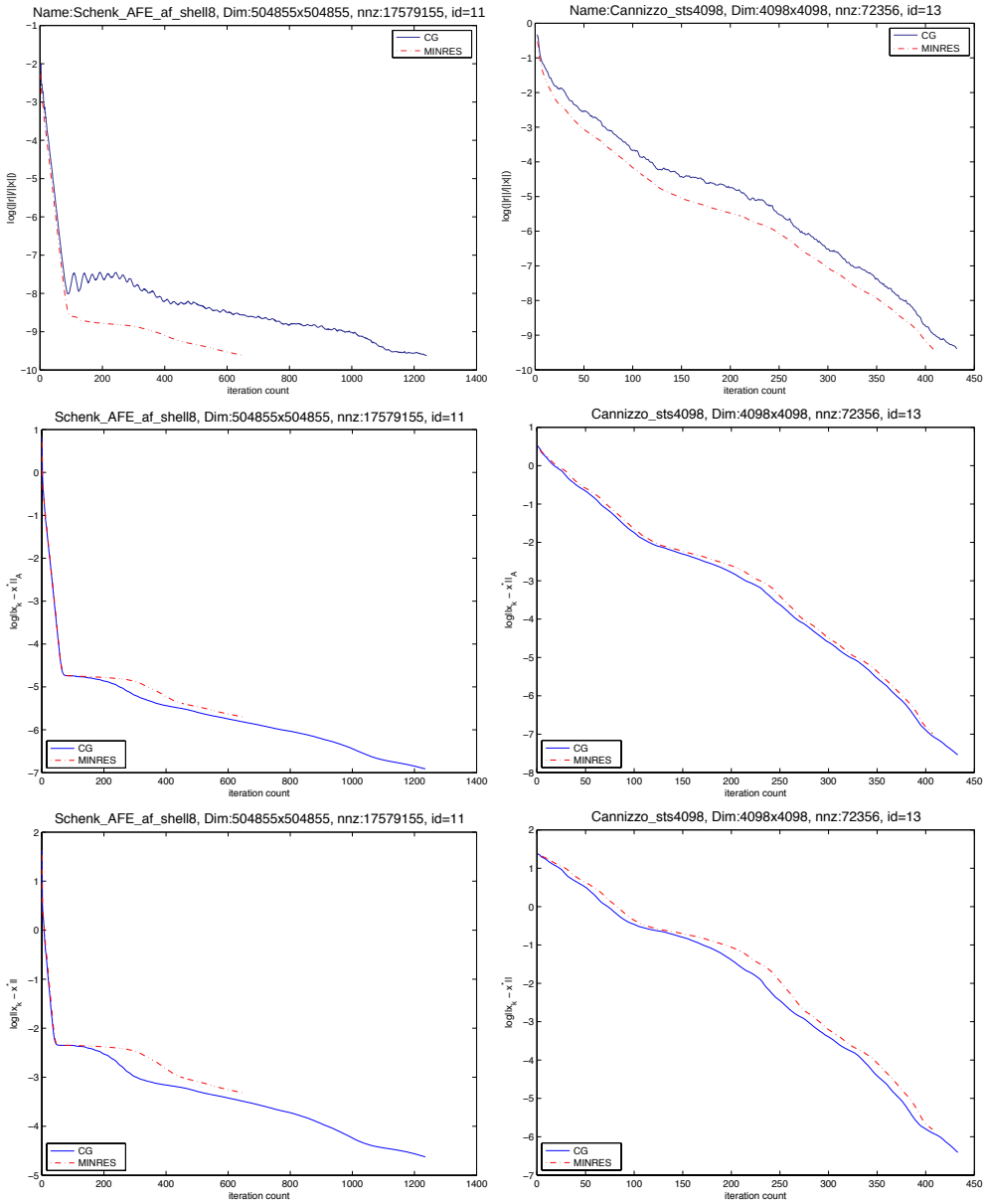

FIG. 4.2. *Comparison of backward and forward errors for CG and MINRES solving two spd systems $Ax = b$.*

***Left**: Problem* `Schenk_AFE_af_shell8` *with $n = 504855$ and cond(A) = 2.7E+05. Note that MINRES stops significantly sooner than CG with $\alpha = 0$ and $\beta = 10^{-8}$ in* (3.4).

***Right**:* `Cannizzo_sts4098` *with $n = 4098$ and cond(A) = 6.7E+03. MINRES stops slightly sooner than CG.*

***Top**: The values of $\log_{10}(\|r_k\|/\|x_k\|)$ are plotted against iteration number k. These values define $\log_{10}(\|E_k\|)$ when the stopping tolerances in* (3.4) *are $\alpha > 0$ and $\beta = 0$.*

***Middle**: The values of $\log_{10}\|x^* - x_k\|_A$ are plotted against iteration number k. This is the quantity that CG minimizes at each iteration.*

***Bottom**: The values of $\log_{10}\|x^* - x_k\|$.*

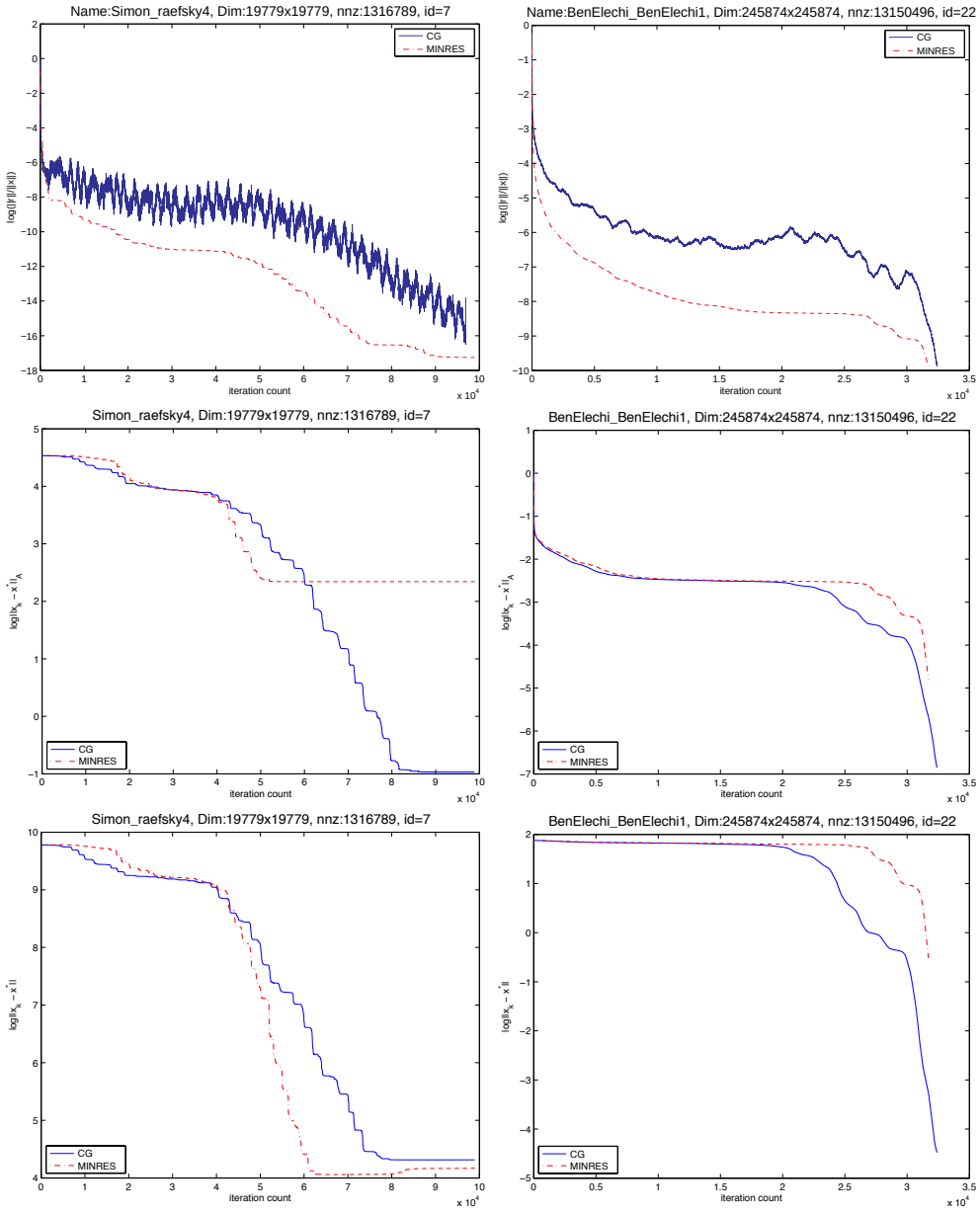

FIG. 4.3. *Comparison of backward and forward errors for CG and MINRES solving two more spd systems $Ax = b$.*

***Left**: Problem* `Simon_raefsky4`*, with $n = 19779$ and cond(A) = 2.2E+11.*

***Right**:* `BenElechi_BenElechi1`*, with $n = 245874$ and cond(A) = 1.8E+09.*

***Top**: The values of $\log_{10}(\|r_k\|/\|x_k\|)$ are plotted against iteration number k. These values define $\log_{10}(\|E_k\|)$ when the stopping tolerances in (3.4) are $\alpha > 0$ and $\beta = 0$.*

***Middle**: The values of $\log_{10}\|x^* - x_k\|_A$ are plotted against iteration number k. This is the quantity that CG minimizes at each iteration.*

***Bottom**: The values of $\log_{10}\|x^* - x_k\|$.*

Figure 4.3 (left) shows problem `Simon_raefsky4` with A of size 19779×19779 and $\text{cond}(A) = 2.2\text{E}{+}11$. Because of the high condition number, both algorithms hit the $5n$ iteration limit. We see that the backward error for MINRES converges faster than for CG as expected. For the energy norm error, CG is able to decrease over 5 orders of magnitude while MINRES plateaus after a 2 orders of magnitude decrease. For both the energy norm error and 2-norm error, MINRES reaches a lower point than CG for some iterations. This must be due to numerical error in CG and MINRES (a result of loss of orthogonality in V_k).

Figure 4.3 (right) shows problem `BenElechi_BenElechi1` with A of size 245874×245874 and $\text{cond}(A) = 1.8\text{E}{+}09$. The backward error of MINRES stays ahead of CG by 2 orders of magnitude for most iterations. Around iteration 32000, the backward error of both algorithms goes down rapidly and CG catches up with MINRES. Both algorithms exhibit a plateau on energy norm error for the first 20000 iterations. The error norms for CG start decreasing around iteration 20000 and decrease even faster after iteration 30000.

Figure 4.4 shows $\|r_k\|$ and $\|x_k\|$ for CG and MINRES on two typical spd examples. We see that $\|x_k\|$ is monotonically increasing for both solvers, and the $\|x_k\|$ values rise fairly rapidly to their limiting value $\|x^*\|$, with a moderate delay for MINRES.

Figure 4.5 shows $\|r_k\|$ and $\|x_k\|$ for CG and MINRES on two spd examples in which the residual decrease and the solution norm increase are somewhat slower than typical. The rise of $\|x_k\|$ for MINRES is rather more delayed. In the second case, if the stopping tolerance were $\beta = 10^{-6}$ rather than $\beta = 10^{-8}$, the final MINRES $\|x_k\|$ ($k \approx 10000$) would be less than half the exact value $\|x^*\|$. It will be of future interest to evaluate this effect within the context of trust-region methods for optimization.

4.1.1. Why does $\|r_k\|$ for CG lag behind MINRES?. It is commonly thought that even though MINRES is known to minimize $\|r_k\|$ at each iteration, the cumulative minimum of $\|r_k\|$ for CG should approximately match that of MINRES. That is,

$$\min_{0 \le i \le k} \|r_i^C\| \approx \|r_k^M\|.$$

However, in Figures 4.2 and 4.3 we see that $\|r_k\|$ for MINRES is often smaller than for CG by 1 or 2 orders of magnitude. This phenomenon can be explained by the following relations between $\|r_k^C\|$ and $\|r_k^M\|$ [10, Lemma 5.4.1] and [26]:

$$\|r_k^C\| = \frac{\|r_k^M\|}{\sqrt{1 - \|r_k^M\|^2 / \|r_{k-1}^M\|^2}}. \tag{4.1}$$

From (4.1), one can infer that if $\|r_k^M\|$ decreases a lot between iterations $k-1$ and k, then $\|r_k^C\|$ would be roughly the same as $\|r_k^M\|$. The converse also holds, in that $\|r_k^C\|$ will be much larger than $\|r_k^M\|$ if MINRES is almost stalling at iteration k (i.e., $\|r_k^M\|$ did not decrease much relative to the previous iteration). The above analysis was pointed out by Titley-Peloquin [26] in comparing LSQR and LSMR [8]. We repeat the analysis here for CG vs MINRES and extend it to demonstrate why there is a lag in general for large problems.

With $\alpha = 0$ in stopping rule (3.4), CG and MINRES stop when $\|r_k\| \le \beta\|b\|$. If this occurs at iteration l, we have

$$\prod_{k=1}^{l} \frac{\|r_k\|}{\|r_{k-1}\|} = \frac{\|r_l\|}{\|b\|} \approx \beta.$$

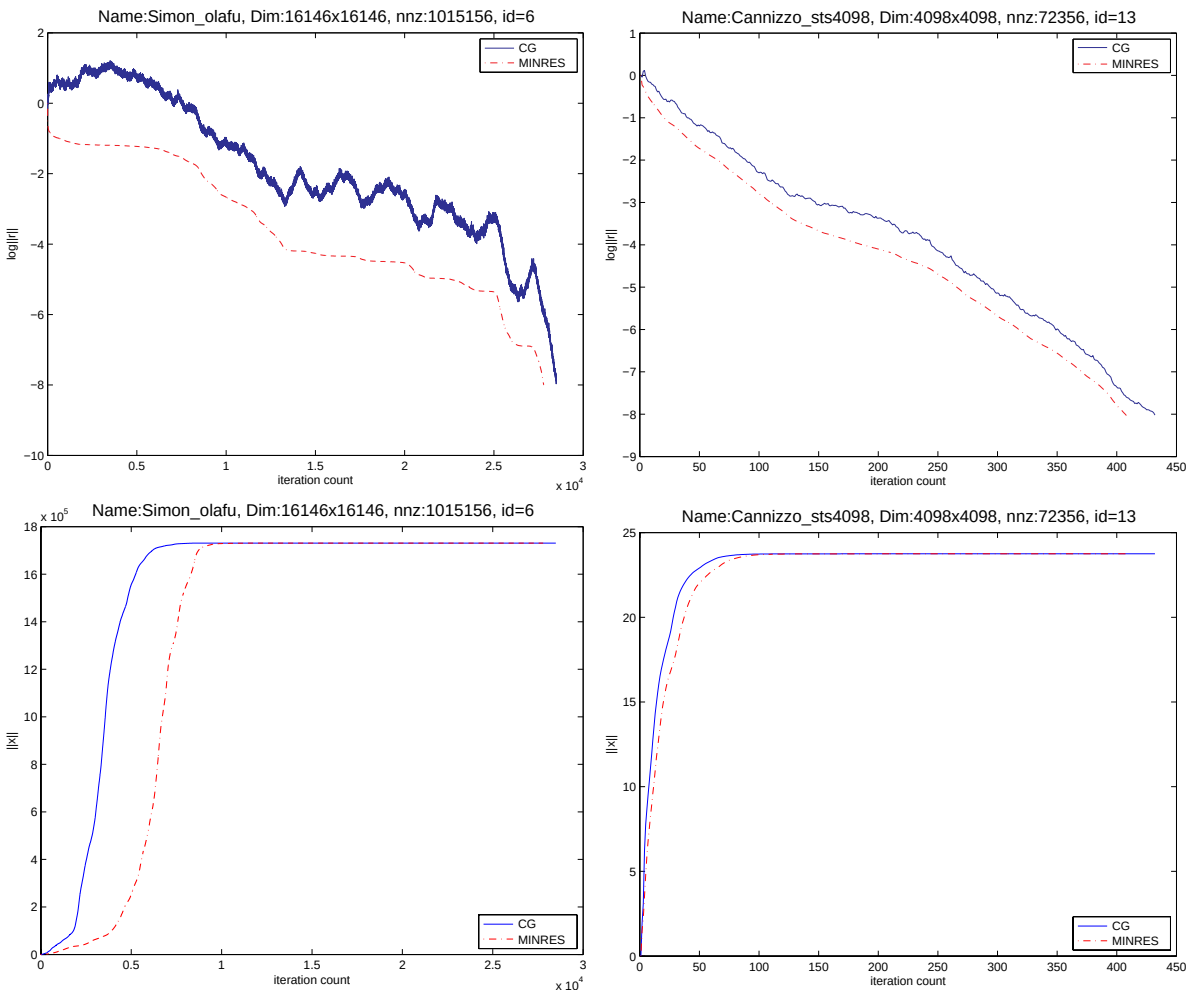

FIG. 4.4. *Comparison of residual and solution norms for CG and MINRES solving two spd systems $Ax = b$. These are typical examples.*

***Left**: Problem* `Simon_olafu` *with $n = 16146$ and cond(A) = 4.3E+08.*

***Right**: Problem* `Cannizzo_sts4098` *with $n = 4098$ and cond(A) = 6.7E+03.*

***Top**: The values of $\log_{10} \|r_k\|$ are plotted against iteration number k.*

***Bottom**: The values of $\|x_k\|$ are plotted against k. The solution norms grow somewhat faster for CG than for MINRES. Both reach the limiting value $\|x^*\|$ significantly before x_k is close to x^*.*

Thus on average, $\|r_k^M\|/\|r_{k-1}^M\|$ will be closer to 1 if l is large. This means that the larger l is (in absolute terms), the more CG will lag behind MINRES (a bigger gap between $\|r_k^C\|$ and $\|r_k^M\|$).

4.2. Indefinite systems. A key part of Steihaug's trust-region method for large-scale unconstrained optimization [21] (see also [4]) is his proof that when CG is applied to a symmetric (possibly indefinite) system $Ax = b$, the solution norms $\|x_1\|, \ldots, \|x_k\|$ are strictly increasing as long as $p_j^T A p_j > 0$ for all iterations $1 \le j \le k$. (We are using the notation in Table 2.1.)

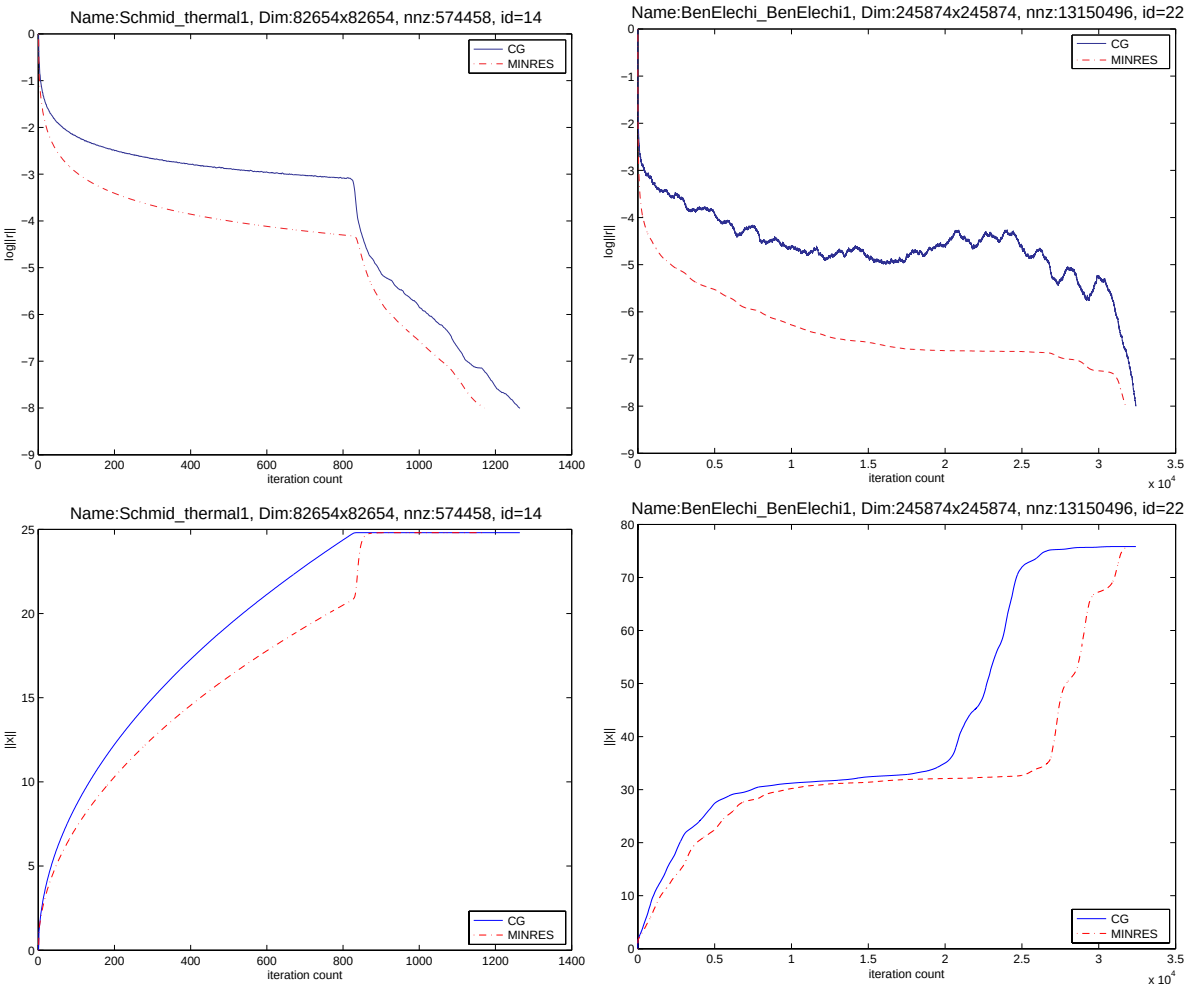

FIG. 4.5. *Comparison of residual and solution norms for CG and MINRES solving two more spd systems $Ax = b$. Sometimes the solution norms take longer to reach the limiting value $\|x^*\|$.*
***Left**: Problem* `Schmid_thermal1` *with $n = 82654$ and cond(A) = 3.0E+05.*
***Right**: Problem* `BenElechi_BenElechi1` *with $n = 245874$ and cond(A) = 1.8E+09.*
***Top**: The values of $\log_{10}\|r_k\|$ are plotted against iteration number k.*
***Bottom**: The values of $\|x_k\|$ are plotted against k. Again the solution norms grow faster for CG.*

From our proof of Theorem 2.2, we see that the same property holds for CR and MINRES as long as both $p_j^T A p_j > 0$ and $r_j^T A r_j > 0$ for all iterations $1 \le j \le k$. In case future research finds that MINRES is a useful solver in the trust-region context, it is of interest now to offer some empirical results about the behavior of $\|x_k\|$ when MINRES is applied to indefinite systems.

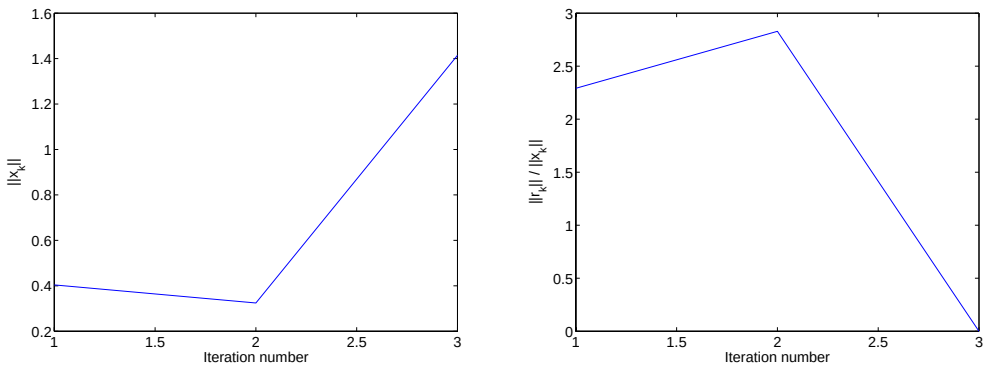

FIG. 4.6. *For MINRES on the indefinite problem* (4.2), $\|x_k\|$ *and the backward error* $\|r_k\|/\|x_k\|$ *are both slightly non-monotonic.*

First, on the nonsingular indefinite system

$$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 2 \end{pmatrix} x = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \tag{4.2}$$

MINRES gives non-monotonic solution norms, as shown in the left plot of Figure 4.6. The decrease in $\|x_k\|$ implies that the backward errors $\|r_k\|/\|x_k\|$ may not be monotonic, as illustrated in the right plot.

More generally, we can gain an impression of the behavior of $\|x_k\|$ by recalling from Choi et al. [3] the connection between MINRES and MINRES-QLP. Both methods compute the iterates $x_k^M = V_k y_k^M$ in (2.1) from the subproblems

$$y_k^M = \arg\min_{y \in \mathbb{R}^k} \|\underline{T_k} y - \beta_1 e_1\| \quad \text{and possibly} \quad T_\ell y_\ell^M = \beta_1 e_1.$$

When A is nonsingular or $Ax = b$ is consistent (which we now assume), y_k^M is uniquely defined for each $k \le \ell$ and the methods compute the same iterates x_k^M (but by different numerical methods). In fact they both compute the expanding QR factorizations

$$Q_k \begin{bmatrix} \underline{T_k} & \beta_1 e_1 \end{bmatrix} = \begin{bmatrix} R_k & t_k \\ 0 & \phi_k \end{bmatrix},$$

(with R_k upper tridiagonal) and MINRES-QLP also computes the orthogonal factorizations $R_k P_k = L_k$ (with L_k lower tridiagonal), from which the kth solution estimate is defined by $W_k = V_k P_k$, $L_k u_k = t_k$, and $x_k^M = W_k u_k$. As shown in [3, §5.3], the construction of these quantities is such that the first $k-3$ columns of W_k are the same as in W_{k-1}, and the first $k-3$ elements of u_k are the same as in u_{k-1}. Since W_k has orthonormal columns, $\|x_k^M\| = \|u_k\|$, where the first $k-2$ elements of u_k are unaltered by later iterations. As shown in [3, §6.5], it means that certain quantities can be cheaply updated to give norm estimates in the form

$$\chi^2 \leftarrow \chi^2 + \hat{\mu}_{k-2}^2, \qquad \|x_k^M\|^2 = \chi^2 + \tilde{\mu}_{k-1}^2 + \bar{\mu}_k^2,$$

where it is clear that χ^2 increases monotonically. Although the last two terms are of unpredictable size, $\|x_k^M\|^2$ tends to be dominated by the monotonic term χ^2 and we can expect that $\|x_k^M\|$ will be *approximately* monotonic as k increases from 1 to ℓ.

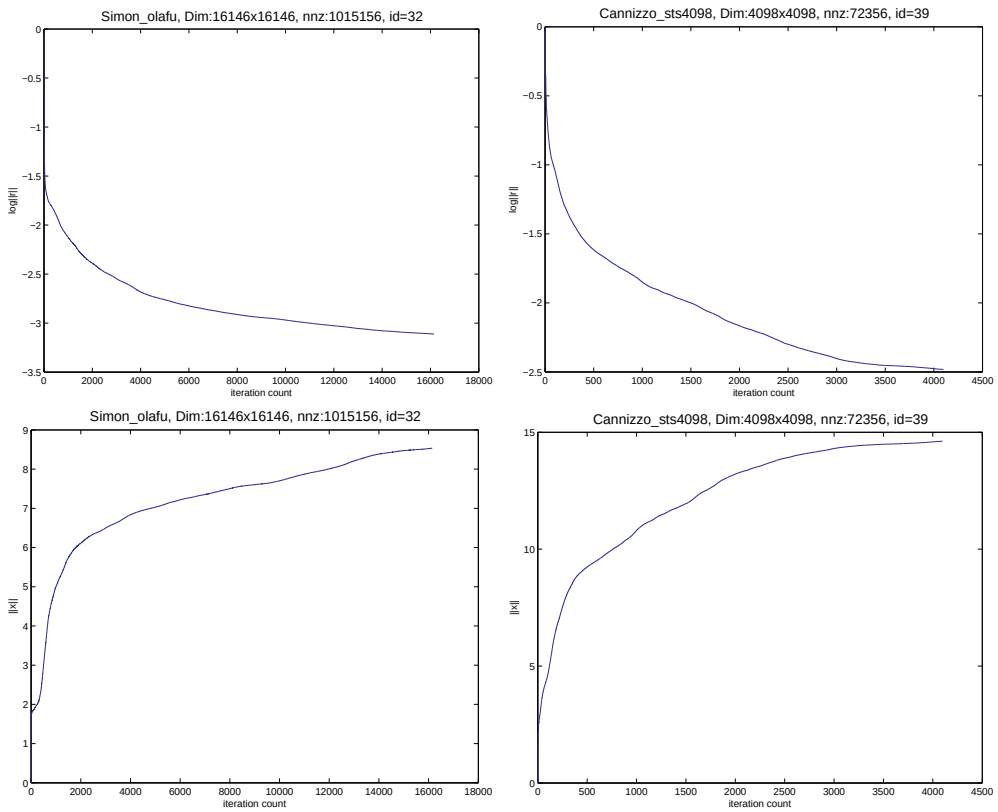

FIG. 4.7. *Residual norms and solution norms when MINRES is applied to two indefinite systems* $(A - \delta I)x = b$*, where* A *is the spd matrices used in Figure 4.4 and* $\delta = 0.5$ *is large enough to make the systems indefinite.*

Left*: Problem* `Simon_olafu` *with* $n = 16146$.

Right*: Problem* `Cannizzo_sts4098` *with* $n = 4098$.

Top*: The values of* $\log_{10} \|r_k\|$ *are plotted against iteration number* k *for the first* n *iterations.*

Bottom left*: The values of* $\|x_k\|$ *are plotted against* k*. During the* $n = 16146$ *iterations,* $\|x_k\|$ *increased 83% of the time and the backward errors* $\|r_k\|/\|x_k\|$ *(not shown) decreased 96% of the time.*

Bottom right*: During the* $n = 4098$ *iterations,* $\|x_k\|$ *increased 90% of the time and the backward errors* $\|r_k\|/\|x_k\|$ *(not shown) decreased 98% of the time.*

Experimentally we find that for most MINRES iterations on an indefinite problem, $\|x_k\|$ does increase. To obtain indefinite examples that were sensibly scaled, we used the four spd (A, b) cases in Figures 4.4–4.5, applied diagonal scaling as before, and solved $(A - \delta I)x = b$ with $\delta = 0.5$ and where A and b are now scaled (so that $\text{diag}(A) = I$). The number of iterations increased significantly but was limited to n.

Figure 4.7 shows $\log_{10} \|r_k\|$ and $\|x_k\|$ for the first two cases (where A is the spd matrices in Figure 4.4). The values of $\|x_k\|$ are *essentially* monotonic. The backward errors $\|r_k\|/\|x_k\|$ (not shown) were even closer to being monotonic (at least for the first n iterations).

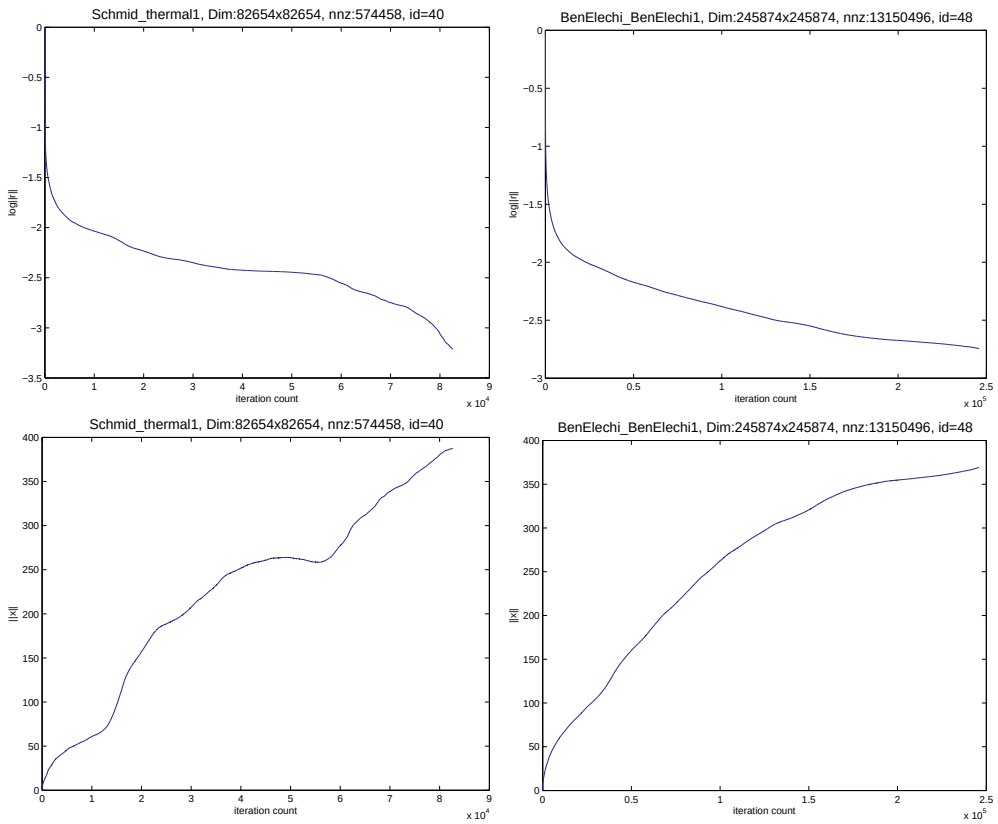

FIG. 4.8. *Residual norms and solution norms when MINRES is applied to two indefinite systems* $(A - \delta I)x = b$*, where* A *is the spd matrices used in Figure 4.5 and* $\delta = 0.5$ *is large enough to make the systems indefinite.*

Left*: Problem* `Schmid_thermal1` *with* $n = 82654$.

Right*: Problem* `BenElechi_BenElechi1` *with* $n = 245874$.

Top*: The values of* $\log_{10} \|r_k\|$ *are plotted against iteration number* k *for the first* n *iterations.*

Bottom left*: The values of* $\|x_k\|$ *are plotted against* k*. There is a mild but clear decrease in* $\|x_k\|$ *over an interval of about 10000 iterations. During the* $n = 82654$ *iterations,* $\|x_k\|$ *increased 83% of the time and the backward errors* $\|r_k\|/\|x_k\|$ *(not shown) decreased 91% of the time.*

Bottom right*: The solution norms and backward errors are essentially monotonic. During the* $n = 245874$ *iterations,* $\|x_k\|$ *increased 88% of the time and the backward errors* $\|r_k\|/\|x_k\|$ *(not shown) decreased 95% of the time.*

Figure 4.8 shows $\|x_k\|$ and $\log_{10} \|r_k\|$ for the second two cases (where A is the spd matrices in Figure 4.5). The left example reveals a definite period of decrease in $\|x_k\|$. Nevertheless, during the $n = 82654$ iterations, $\|x_k\|$ increased 83% of the time and the backward errors $\|r_k\|/\|x_k\|$ decreased 91% of the time. The right example is more like those in Figure 4.7. During $n = 245874$ iterations, $\|x_k\|$ increased 83% of the time, the backward errors $\|r_k\|/\|x_k\|$ decreased 91% of the time, and any nonmonotonicity was very slight.

TABLE 5.1
Comparison of CG and MINRES properties on an spd system $Ax = b$.

	CG	MINRES
$\|x_k\|$	$\nearrow$ [21, Thm 2.1]	$\nearrow$ (Thm 2.3)
$\|x^* - x_k\|$	$\searrow$ [11, Thm 4:3]	$\searrow$ (Thm 2.4) [11, Thm 7:5]
$\|x^* - x_k\|_A$	$\searrow$ [11, Thm 6:3]	$\searrow$ (Thm 2.5) [11, Thm 7:4]
$\|r_k\|$	not-monotonic	$\searrow$ [18] [11, Thm 7:2]
$\|r_k\|/\|x_k\|$	not-monotonic	$\searrow$ (Thm 3.1)

$\nearrow$ monotonically increasing
$\searrow$ monotonically decreasing

TABLE 5.2
Comparison of LSQR and LSMR properties on $\min \|Ax - b\|$.

	LSQR	LSMR
$\|x_k\|$	$\nearrow$ [7, Thm 3.3.1]	$\nearrow$ [7, Thm 3.3.6]
$\|x^* - x_k\|$	$\searrow$ [7, Thm 3.3.2]	$\searrow$ [7, Thm 3.3.7]
$\|r^* - r_k\|$	$\searrow$ [7, Thm 3.3.3]	$\searrow$ [7, Thm 3.3.8]
$\|A^T r_k\|$	not-monotonic	$\searrow$ [8, §3.2]
$\|r_k\|$	$\searrow$ [19, §5.1]	$\searrow$ [7, Thm 3.3.11]
	$(\|A^T r_k\|/\|r_k\|)^{\text{LSQR}} \geq (\|A^T r_k\|/\|r_k\|)^{\text{LSMR}}$	
x_k converges to minimum-norm x^* for singular systems		

5. Conclusions. For full-rank least-squares problems $\min \|Ax - b\|$, the solvers LSQR [19, 20] and LSMR [8, 14] are equivalent to CG and MINRES on the (spd) normal equation $A^T Ax = A^T b$. Comparisons in [8] indicated that LSMR can often stop much sooner than LSQR when the stopping rule is based on Stewart's backward error norm $\|A^T r_k\|/\|r_k\|$ for least-squares problems [22].

Our theoretical and experimental results here provide analogous evidence that MINRES can often stop much sooner than CG on spd systems when the stopping rule is based on the backward error $\|r_k\|/\|x_k\|$ for $Ax = b$ (or the more general backward errors in Theorem 3.1). In some cases, MINRES can converge faster than CG by as much as 2 orders of magnitude (Figure 4.3). On the other hand, CG converges somewhat faster than MINRES in terms of both $\|x^* - x_k\|_A$ and $\|x^* - x_k\|$ (same figure). For spd systems, Table 5.1 summarizes properties that were already known by Hestenes and Stiefel [11] and Steihaug [21], along with the two additional properties of MINRES that we proved here (Theorems 2.3 and 3.1).

These theorems and experiments on CG and MINRES are part of the first author's PhD thesis [7], which also discusses LSQR and LSMR and derives some new results for both solvers. Table 5.2 summarizes the known results for LSQR and LSMR (in [19] and [8] respectively) and the newly derived properties for both solvers (in [7]).

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