

Iterative methods for solving $Ax = b$, GMRES/FOM versus QMR/BiCG*

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We study the convergence of the GMRES/FOM and QMR/BiCG methods for solving non-symmetric systems of equations $Ax = b$. We prove, in exact arithmetic, that any type of residual norm convergence obtained using BiCG can also be obtained using FOM but on a different system of equations. We consider practical comparisons of these procedures when they are applied to the same matrices. We use a unitary invariance shared by both methods, to construct test matrices where we can vary the nonnormality of the test matrix by variations in simplified eigenvector matrices. We used these test problems in two sets of numerical experiments. The first set of experiments was designed to study effects of increasing nonnormality on the convergence of GMRES and QMR. The second set of experiments was designed to track effects of the eigenvalue distribution on the convergence of QMR. In these tests the GMRES residual norms decreased significantly more rapidly than the QMR residual norms but without corresponding decreases in the error norms. Furthermore, as the nonnormality of A was increased, the GMRES residual norms decreased more rapidly. This led to premature termination of the GMRES procedure on highly nonnormal problems. On the nonnormal test problems the QMR residual norms exhibited less sensitivity to changes in the nonnormality. The convergence of either type of procedure, as measured by the error norms, was delayed by the presence of large or small outliers and affected by the type of eigenvalues, real or complex, in the eigenvalue distribution of A . For GMRES this effect can be seen only in the error norm plots.

1. Introduction

Computer simulation is an integral part of the analysis of physical phenomena and of the successful design and implementation of many systems and structures. Simulations

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require realistic mathematical models and practical numerical algorithms. Model complexity may be limited by the types of algorithms which are available. Many computer simulations require the repeated solution of large systems of linear equations

$$Ax = b. \quad (1)$$

Often these systems are too large for numerical methods which explicitly modify the matrix, and it becomes necessary to use iterative methods which obtain information about the problem through a sequence of matrix–vector computations.

Much of the current research on iterative methods for solving nonsymmetric equation (1) focuses on two sets of Krylov subspace methods and their variants. Each set is based upon recursions which, in exact arithmetic, map the matrix A into a family of projection matrices which are then used to obtain approximations to a solution of equation (1). The first set of methods is based upon the Arnoldi recursion and includes the generalized minimal residual method (GMRES), the full orthogonal method (FOM), and their variants such as restarted GMRES(q) [24]. The second set of methods is based upon nonsymmetric Lanczos recursions, and includes the bi-conjugate gradient method (BiCG), the quasi-minimal residual method (QMR), and their variants such as BiCGSTAB(q) [15, 31, 20, 30].

In this paper we study the convergence behavior of the GMRES/FOM and QMR/BiCG methods. In section 2 we summarize these methods. In section 3, assuming exact arithmetic, we prove that any type of residual norm behavior which can be obtained using the BiCG method on equation (1) can be obtained using the FOM method on a different equation. We obtain a similar result for QMR and GMRES but involving the GMRES residual norms and the QMR quasi-residual norms.

In practical situations we are not interested in comparisons of methods across different problems but in comparisons on the same problems. Therefore, in section 4 we consider the design of sets of experiments for obtaining such comparisons. We use a unitary equivalence shared by both methods to construct test matrices where we can vary the nonnormality of the test matrices by variations in simplified eigenvector matrices. We present a mechanism for maintaining consistency in tests across changes in nonnormality or changes in the eigenvalue distribution of A . In section 5 we use these test matrices in two sets of numerical experiments. The first set of experiments is designed to study effects of increasing nonnormality on the convergence of QMR and GMRES. The second set of experiments is designed to track effects of the eigenvalue distribution on the convergence of QMR for normal and for nonnormal matrices. The tests in section 5 use the MATLAB [21] templates discussed in [1].

The topics addressed are of major interest to algorithm developers and to users of iterative methods. In the literature we find several interesting discussions of observed behavior of iterative methods on nonnormal matrices. See, for example, [8, 7, 3, 2, 28, 27, 6]. These papers focus on relationships between the nonnormality of a matrix and the observed convergence or nonconvergence of various iterative methods, and on mechanisms for identifying and characterizing nonnormality. The importance of the pseudospectra for the convergence of iterative methods for $Ax = b$ with nonnormal A was first discussed in [29, 22].

We use the following notation.

1.1. Notation

$A = (a_{ij})$, $1 \leq i, j \leq n$, $n \times n$ matrix,
 $A^T = (a_{ji})$, transpose of A , $A^H = (\bar{a}_{ji})$, complex conjugate transpose of A ,
 $D = \text{diag}\{d_1, \dots, d_n\}$, $n \times n$ diagonal matrix
 $\lambda_j(A)$, $1 \leq j \leq n$, eigenvalues of A , $w(A) = \{\lambda_j(A), 1 \leq j \leq n\}$,
 $\sigma_j(A)$, $1 \leq j \leq n$, singular values of A where $\sigma_1 \geq \dots \geq \sigma_n$, $\Sigma = \text{diag}\{\sigma_1, \dots, \sigma_n\}$,
 $\kappa(A) = \sigma_{\max}(A)/\sigma_{\min}(A)$, condition number of A ,
 $\|A\| = \sigma_{\max}(A)$, $\|x\| = \sqrt{\sum_{j=1}^n x_j^2}$,
 $\mathcal{K}_j(A, b) = \text{span}\{b, Ab, \dots, A^{j-1}b\}$, j th Krylov subspace generated by A and b ,
 v_j , j th vector in any sequence of vectors, $V_j = \{v_1, \dots, v_j\}$,
 x_j^M = j th iterate, $\varepsilon_j^M = x_j^M - x_{\text{true}}$ true error, $\delta_j^M = x_j^M - x_0$ for method M ,
 $r_j^M = -Ax_j^M + b = -A\delta_j^M + r_0$, j th residual vector corresponding to x_j^M and δ_j^M ,
 \mathbb{R}^m , m -dimensional Euclidean space, e_j , j th coordinate vector in \mathbb{R}^m ,
 \hat{e}_j , j th coordinate vector in \mathbb{R}^{m+1} where m is specified in the context,
 I_j , $j \times j$ identity matrix,
 A , C subscripts denote respectively a matrix A , C ,
 B , F , Q , G superscripts denote respectively, BiCG, FOM, QMR, GMRES quantities.

2. Krylov subspace methods: GMRES/FOM and QMR/BiCG

In this section we summarize the GMRES/FOM and QMR/BiCG methods. Without loss of generality we can consider the equivalent system $A\delta = r_0$ where $r_0 = -Ax_0 + b$ and $\delta = x_{\text{true}} - x_0$.

2.1. Arnoldi methods: GMRES/FOM

The GMRES, FOM, and GMRES(q) methods are based upon the Arnoldi recursion [24–26]. In exact arithmetic, for a given matrix A and a given starting vector v_1 , the Arnoldi recursion generates orthonormal bases $V_j = \{v_1, \dots, v_j\}$, $j = 1, 2, \dots$, for the Krylov subspaces $\mathcal{K}_j(A, v_1)$, and Hessenberg matrices $H_j \equiv (h_{ik})$, $1 \leq i, k \leq j$, which are matrix representations, with respect to the bases V_j , of the orthogonal projections of A on these subspaces.

Arnoldi recursion:

1. Specify v_1 with $\|v_1\| = 1$. For $j = 2, 3, \dots$ compute $v_{j+1} = Av_j$.
2. For each j and for $i = 1, \dots, j$ compute $h_{ij} = v_i^H v_{j+1}$, $v_{j+1} = v_{j+1} - h_{ij}v_i$.

3. For each j compute $h_{j+1,j} = \|v_{j+1}\|$ and $v_{j+1} = v_{j+1}/h_{j+1,j}$.

The preceding implementation uses modified Gram–Schmidt orthogonalization [19]. Other implementations exist [32]. In matrix form these recursions become

$$AV_j = V_j H_j + h_{j+1,j} v_{j+1} e_j^T$$

or

$$AV_j = V_{j+1} H_j^{(e)} \quad \text{where } H_j^{(e)} = \begin{pmatrix} H_j \\ h_{j+1,j} e_j^T \end{pmatrix}. \quad (2)$$

2.2. GMRES/FOM

In GMRES and FOM, the starting vector $v_1 \equiv r_0/\|r_0\|$. In exact arithmetic, at each iteration j , GMRES and FOM select their iterates, δ_j^G , δ_j^F , from the same Krylov subspaces but subject to different constraints on the corresponding residual vectors, r_j^G and r_j^F .

In GMRES each iterate is selected so that the norm of the corresponding residual vector, r_j^G , is minimal over the j th Krylov subspace $\mathcal{K}_j(A, r_0)$. For each j ,

$$\|r_j^G\| = \min_{\delta \in \mathcal{K}_j(A, r_0)} \|r_0 - A\delta\| = \|r_0 - A\delta_j^G\|$$

or equivalently

$$r_j^G \perp AK_j(A, r_0). \quad (3)$$

Using equation (2), constraint (3), and the orthonormality of the Arnoldi vectors, it is not difficult to prove that in exact arithmetic the j th GMRES iterate

$$\delta_j^G = V_j y_j^G \quad \text{where } y_j^G \text{ satisfies } \min_y \| -H_j^{(e)} y + \|r_0\| \widehat{e}_1 \|. \quad (4)$$

In FOM each iterate is selected so that the corresponding residual vector, r_j^F , is orthogonal to the j th Krylov subspace $\mathcal{K}_j(A, r_0)$ [24, 26]. For each j ,

$$r_j^F \perp \mathcal{K}_j(A, r_0). \quad (5)$$

Using equation (2), the constraint (5), and the orthonormality of the Arnoldi vectors, it is not difficult to prove that the j th FOM iterate

$$\delta_j^F = V_j y_j^F \quad \text{where } H_j y_j^F = \|r_0\| e_1. \quad (6)$$

Therefore, each FOM iterate is obtained by solving a system of equations defined by a Galerkin iteration matrix H_j , and each GMRES iterate is obtained by solving a least squares problem defined by H_j^e . We cannot guarantee that the Galerkin equations are well-conditioned or even nonsingular. If H_j is singular for some j , then the j th FOM iterate would not be defined but if this occurs, the corresponding j th GMRES iterate is identical to the $(j-1)$ -th GMRES iterate [5]. We have the following lemma.

Lemma 2.1 (Exact arithmetic). Apply GMRES/FOM to equation (1). For each j , define the quasi-residual vector $z_j^{G,F} \equiv -H_j^e y_j^{G,F} + \|r_0\| \widehat{e}_1$. Set $\delta_j^{G,F} \equiv V_j^{G,F} y_j^{G,F}$, then the corresponding residual vectors

$$r_j^{G,F} \equiv -A\delta_j^{G,F} + r_0 = V_{j+1}^{G,F} z_j^{G,F} \quad \text{and} \quad \|r_j^{G,F}\| = \|z_j^{G,F}\|. \quad (7)$$

For any $1 \leq q \leq n$, GMRES(q) is GMRES restarted with the current residual vector after each q iterations [24].

2.3. Nonsymmetric Lanczos methods: QMR/BiCG

The QMR, BiCG, and BiCGSTAB(q) methods are based upon nonsymmetric Lanczos recursions. We need the following definition.

Definition 2.2. Two sets of vectors, $V_j = \{v_1, \dots, v_j\}$ and $W_j = \{w_1, \dots, w_j\}$ are said to be *complex bi-orthogonal* if and only if $W_j^T V_j = D_j$ where D_j is a nonsingular diagonal matrix [23].

For a given matrix A and for given starting vectors v_1, w_1 , the coefficients in any nonsymmetric Lanczos recursions are chosen so that two sets of Lanczos vectors, $V_j = \{v_1, \dots, v_j\}$ and $W_j = \{w_1, \dots, w_j\}$, $j = 1, 2, \dots$, satisfy the following conditions. For each j , V_j is a basis for the Krylov subspace $\mathcal{K}_j(A, v_1)$, W_j is a basis for the Krylov subspace $\mathcal{K}_j(A^T, w_1)$, and these bases are complex bi-orthogonal. The coefficients define tridiagonal matrices T_j such that for each j , $T_j \equiv W_j^T A V_j$ is a matrix representation of the oblique projection of A onto $\mathcal{K}_j(A, v_1)$ along $\mathcal{K}_j(A^T, w_1)$ [24]. We use the following recursions where the Lanczos vectors are scaled to have unit norms [15]. Other variants are discussed in [23, 12, 24].

Nonsymmetric Lanczos recursion:

1. Specify v_1 and w_1 with $\|w_1\| = \|v_1\| = 1$. Set $v_0 = w_0 = 0$ and $\beta_1 = 0$. Set $\rho_1 = \xi_1 = 1$.
2. For each $i = 1, \dots, j$ compute

$$\begin{aligned}
 v_{i+1} &= A v_i \quad \text{and} \quad w_{i+1} = A^T w_i, \\
 \alpha_i &= w_i^T v_{i+1} / w_i^T v_i, \\
 p_i &= v_{i+1} - \alpha_i v_i - \beta_i v_{i-1}, \\
 s_i &= w_{i+1} - \alpha_i w_i - (\beta_i \rho_i / \xi_i) w_{i-1}, \\
 \rho_{i+1} &= \|p_i\|, \quad v_{i+1} = p_i / \rho_{i+1}, \\
 \xi_{i+1} &= \|s_i\|, \quad w_{i+1} = s_i / \xi_{i+1}, \\
 \beta_{i+1} &= \xi_{i+1} w_{i+1}^T v_{i+1} / w_i^T v_i.
 \end{aligned} \tag{8}$$

In matrix form these recursions can be written as

$$\begin{aligned}
 A V_j &= V_j T_j + \gamma_{j+1} v_{j+1} e_j^T \\
 A^T W_j &= W_j \tilde{T}_j + \omega_{j+1} w_{j+1} e_j^T
 \end{aligned}
 \quad \text{or equivalently} \quad
 \begin{aligned}
 A V_j &= V_{j+1} T_j^{(e)} \\
 A^T W_j &= W_{j+1} \tilde{T}_j^{(e)},
 \end{aligned} \tag{9}$$

where

$$\begin{aligned}
 T_j^{(e)} &\equiv \begin{pmatrix} T_j \\ \rho_{j+1} e_j^T \end{pmatrix}, \quad \tilde{T}_j = \Phi_j^{-1} T_j \Phi_j, \\
 \Phi_j &= \text{diag}(\phi_1, \dots, \phi_j), \quad \phi_1 = 1, \quad \phi_j = \phi_{j-1} \rho_j / \xi_j,
 \end{aligned}$$

and

$$T_j = \begin{pmatrix} \alpha_1 & \beta_2 & & & \\ \rho_2 & \alpha_2 & \beta_3 & & \\ & \rho_3 & \ddots & \ddots & \\ & & \ddots & \alpha_{j-1} & \beta_j \\ & & & \rho_j & \alpha_j \end{pmatrix}. \tag{10}$$

2.4. QMR/BiCG

In exact arithmetic QMR and BiCG select their iterates, δ_j^Q , δ_j^B , from the same Krylov subspaces as GMRES and FOM but subject to different constraints on the residual vectors.

QMR is a direct analog of GMRES. In QMR each iterate is chosen so that

$$\delta_j^Q = V_j y_j^Q \quad \text{where } z_j^Q \equiv -T_j^{(e)} y_j^Q + \|r_0\| \hat{e}_1 \text{ satisfies } \min \| -T_j^{(e)} y + \|r_0\| \hat{e}_1 \|. \quad (11)$$

Analogous to lemma 2.1 we have that $r_j^Q = V_{j+1}^Q z_j^Q$. However, since the Lanczos vectors V_{j+1}^Q are not orthonormal, the norms of the true residuals in QMR need not be equal to the norms of the quasi-residuals. Since by construction the Lanczos vectors have unit norm, in exact arithmetic we have, see [15, 13],

$$\|r_j^Q\| \leq \sqrt{j+1} \|z_j^Q\|. \quad (12)$$

In practice we observe that $\|r_j^Q\|$ and $\|z_j^Q\|$ appear to track each other until the limits of convergence are achieved. See, for example, [10, figures 1 and 2].

BiCG and FOM are similar but not direct analogs. In BiCG each iterate is chosen so that the j th residual vector, r_j^B , is orthogonal to the j th Krylov subspace generated by A^T and the specified \tilde{r}_0 :

$$r_j^B \perp \mathcal{K}_j(A^T, \tilde{r}_0). \quad (13)$$

Using equations (9), the constraint (13), and the bi-orthogonality of the Lanczos vectors, it is not difficult to prove that the j th BiCG iterate

$$\delta_j^B = V_j y_j^B \quad \text{where } T_j y_j^B = \|r_0\| e_1. \quad (14)$$

Therefore, each BiCG iterate is obtained by solving a system of equations defined by Galerkin iteration matrices T_j , and each QMR iterate is obtained by solving a least squares problem defined by a T_j^e . We cannot guarantee that the Galerkin equations are well-conditioned or even nonsingular. If T_j is singular for some j , then the j th BiCG iterate would not be defined but if this occurs, the corresponding j th QMR iterate is identical to the $(j-1)$ -th QMR iterate [15]. BiCGSTAB(q) are variants of BiCG which do not require A^T and which incorporate GMRES polynomials to accelerate the convergence. For details on their construction see [31, 30].

2.5. Both types of methods

For a given problem, QMR/BiCG and GMRES/FOM select their iterates from the same Krylov subspaces but subject to different constraints on the residual vectors. The methods also differ in their storage requirements and the amount of work required at each iteration. QMR and BiCG require matrix–vector multiplications by A and by A^T but have minimal additional storage requirements. GMRES and FOM require only

A but at each iteration also requires access to all of the previously-generated Arnoldi vectors.

In exact arithmetic, the recursions underlying GMRES/FOM cannot break down. However, even in exact arithmetic, the recursions underlying QMR/BiCG will break down if at some stage in the underlying Lanczos recursions, a bi-orthogonality term $p_j s_j = 0$ for some $p_j \neq 0$ and $s_j \neq 0$. If this occurs then the QMR/BiCG procedures cannot be continued. Exact breakdown is unlikely, near breakdowns can cause numerical instabilities. To avoid such problems, various look-ahead strategies have been proposed, see, for example, [23, 13, 4]. The discussions in this paper are equally applicable to the look-ahead variants of these methods. However, the MATLAB implementations which we use do not include look-ahead heuristics. In addition the Galerkin methods, BiCG and FOM, can experience numerical problems if an iteration matrix, T_j or H_j , is singular or nearly singular.

Typically, in practice, the convergence of a Krylov iterative method is monitored using estimates of the scaled residual norms $\|r_j\|/\|r_0\|$. Recursions (2) and (9) can be used to obtain estimates of the residual norms generated by any of these methods. In exact arithmetic at iteration j

$$\|r_j^{Q,B}\| = \|\rho_{j+1} y_j^{Q,B}(j) v_{j+1}^{Q,B}\| \quad \text{and} \quad \|r_j^{G,F}\| = \|h_{j+1,j} y_j^{G,F}(j) v_{j+1}^{G,F}\|, \quad (15)$$

where $y_j^{Q,B,G,F}(j)$ denotes the j th component of the vector $y_j^{Q,B,G,F}$. Since by construction $\|v_{j+1}^{Q,B,G,F}\| = 1$, we can estimate the norms of the residuals in GMRES, FOM, QMR, or BiCG without computing the true residuals. In finite precision arithmetic, these estimates will be valid as long as the errors in the associated recursions are sufficiently small.

Assumption 2.3. In any statement or theorem about any of these methods we will always assume that no breakdown has occurred, that all quantities are well-defined, and that premature termination of the recursions does not occur.

3. A relationship between BiCG and FOM

The GMRES/FOM methods are orthogonal projection methods. The QMR/BiCG methods are oblique projection methods [24]. In this section we derive a relationship between the BiCG and the FOM methods. We prove, in exact arithmetic, that any type of residual norm behavior obtained using BiCG can also be obtained using FOM on some other problem with the same eigenvalues. The extension of this result to QMR and GMRES establishes a relationship between quasi-residual norms generated by QMR and residual norms generated by GMRES.

Theorem 3.1 (Exact arithmetic). Let A be any $n \times n$ matrix with distinct eigenvalues. Apply BiCG/QMR to $Ax = b$. For $j = 1, \dots, n$,

$$AV_j^{Q,B} = V_j^{Q,B} (T_j^B)^e, \quad (16)$$

where $V_j^{Q,B}$ and $(T_j^B)^e$ denote respectively the Lanczos vectors and matrices generated with $v_1^{Q,B} = r_0/\|r_0\| = w_1^{Q,B} = \tilde{r}_0/\|\tilde{r}_0\|$. Then there exists an $n \times n$ matrix C with the same eigenvalues as A and a vector c such that an application of the FOM/GMRES methods to $Cx = c$ yields

$$\|r_{jC}^F\| = \|z_{jC}^F\| = \|z_{jA}^B\| = \|r_{jA}^B\| \quad \text{for } 1 \leq j \leq n, \quad (17)$$

where z_{jA}^B and z_{jC}^F are the corresponding quasi-residual vectors for BiCG on A and FOM on C . Furthermore,

$$\|r_{jC}^G\| = \|z_{jC}^G\| = \|z_{jA}^Q\|, \quad (18)$$

where z_{jA}^Q and z_{jC}^G are the corresponding quasi-residual vectors for QMR on A and GMRES on C .

Proof. Clearly, the eigenvalues of T_n are equal to the eigenvalues of A . Let

$$T_n^B = Q_n U_n Q_n^H \quad (19)$$

be any Schur decomposition of T_n^B . Define $V_n^F \equiv Q_n^H$, then

$$U_n V_n^F = V_n^F T_n^B. \quad (20)$$

Set $C = U_n$ and c equal to the first column of V_n^F scaled by $\|r_0\|$. Then for each j , V_j^F are FOM vectors corresponding to

$$Cx = c \quad \text{with } H_{jC}^F = T_j^B. \quad (21)$$

Therefore, with y_j^B and z_{jA}^B and z_{jC}^F defined by

$$T_j^B y_j^B = \|r_0\| e_1 \quad \text{and} \quad z_{jA}^B = z_{jC}^F = -(T_j^B)^e y_j^B + \|r_0\| \hat{e}_1, \quad (22)$$

we obtain

$$r_{jC}^F = V_{j+1}^F z_{jC}^F = V_{j+1}^F z_{jA}^B = -\rho_{j+1} y_j^B(j) v_{j+1}^F. \quad (23)$$

Similarly, we have that

$$r_{jA}^B = V_{j+1}^B z_{jA}^B = -\rho_{j+1} v_{j+1}^B y_j^B(j). \quad (24)$$

Therefore, from equations (23) and (24), the fact that $\|v_{j+1}^B\| = 1$, and the orthonormality of the columns of V_j^F ,

$$\|r_{jC}^F\| = \|z_{jC}^F\| = \|z_{jA}^B\| = \|r_{jA}^B\| = |\rho_{j+1} y_j^B(j)|. \quad (25)$$

Equation (18) follows from a similar argument which yields

$$r_{jC}^G = V_{j+1}^F z_{jC}^G \quad \text{and} \quad z_{jC}^G = z_{jA}^Q. \quad (26)$$

Theorem 3.1 states that any portions of the corresponding BiCG and FOM residual norms plots are identical. If we do not require the eigenvalues of C to be equal to the eigenvalues of A , then theorem 3.1 would be applicable to any portion of a BiCG computation in finite precision for which the BiCG residual norms are not too small and the errors in the recursions are sufficiently small. If A has fewer than n distinct eigenvalues, either type of recursions will terminate for some $m < n$ and theorem 3.1 would have to be expressed in terms of m and the distinct eigenvalues of A .

Although in [17] the authors do not consider comparisons between methods, their results can be combined with the results in [9] to obtain a different proof of theorem 3.1 [16]. In [17] the discussions focus on GMRES. The authors prove that given any set of n positive numbers which are ordered from largest to smallest, they can construct $\{C, c\}$ such that C has any specified eigenvalues and when the GMRES method is applied to $Cx = c$, the norms of the residuals generated will match the sequence of positive numbers. [9] considers relationships between residual norms generated within each pair of methods GMRES/FOM and QMR/BiCG and obtains the following theorem. For specific assumptions and proofs see [9].

Theorem 3.2 [9]. In exact arithmetic, the residual norms obtained by applications of GMRES and FOM to $Ax = b$ satisfy

$$\|r_j^F\| = \frac{\|r_j^G\|}{\sqrt{1 - (\|r_j^G\|/\|r_{j-1}^G\|)^2}}. \quad (27)$$

Similarly, in exact arithmetic, the BiCG residual norms and the QMR quasi-residual norms obtained by applications of BiCG and QMR to $Ax = b$ satisfy

$$\|r_j^B\| = \frac{\|z_j^Q\|}{\sqrt{1 - (\|z_j^Q\|/\|z_{j-1}^Q\|)^2}}. \quad (28)$$

We can combine the results in [17, 9] to obtain theorem 3.1. If we are given residual norms generated by a BiCG computation on $Ax = b$, a corresponding application of QMR to this problem yields quasi-residual norms which must be related to the corresponding BiCG residual norms by equation (28). From [17] we can obtain $Cx = c$ with the same eigenvalues as A such that an application of GMRES to $Cx = c$ yields residual norms equal to the QMR quasi-residual norms, equation (18). Then we can apply equation (27) to obtain the corresponding FOM residual norms for $Cx = c$. However, since $\|z_{jC}^G\| = \|r_{jC}^G\| = \|z_{jA}^Q\|$, from equations (27) and (28) we immediately get equation (17) in theorem 3.1.

4. Design of numerical experiments

Theorem 3.1 is an interesting result. However, in practice we are interested in the behavior of these two types of procedures when they are applied to the same problems.

There are several issues to consider in the design of experiments for making such comparisons. How do we measure convergence behavior? Must we consider all of the four methods in our comparisons? What set of test matrices should we use? How should we choose the right-hand sides b ? What software implementations of these procedures should we use?

For the tests in this paper we made the following choices. However, we do not maintain that these are necessarily the only or the correct choices to make. We believe that more discussion on this matter is needed. Our tests were limited and intended only to initiate more discussion on the merits and demerits of each procedure and on the design of such experiments.

4.1. How do we measure convergence behavior?

We track convergence of each procedure by tracking the actual residual norms. We terminate each procedure when $\|r_j\|/\|r_0\| \leq 10^{-12}$. In each test we also compute the true error norms, $\|x_j - x_{\text{true}}\|$, at each iteration.

4.2. Must we consider all four methods?

The relationships in equations (27) and (28) infer that if the GMRES residual norms are decreasing rapidly, then the FOM residual norms must also be decreasing rapidly. Moreover, if the FOM residual norm plot is increasing, then the GMRES residual norm plot must be leveling off. Therefore, if we consider convergence of these procedures to the limits allowed by the finite precision arithmetic, GMRES does not converge more quickly than FOM does. The corresponding statement for QMR/BiCG is between the QMR quasi-residual norms and the BiCG residual norms. Based upon these relationships we consider only the QMR and the GMRES methods in the numerical experiments in this paper.

4.3. What set of test matrices should we use?

We are interested in comparing the behavior of these two types of procedures on the same matrices across changes in nonnormality and in the eigenvalue distribution. It is straightforward to obtain the following unitary invariance for QMR/BiCG, and an analogous theorem for GMRES/FOM.

Theorem 4.1 (Exact arithmetic) (QMR/BiCG). Let U be any unitary matrix. For any A define $C \equiv U^H A U$. For $j = 1, \dots, J$, let T_{jA} , T_{jC} and V_{jA} , W_{jA} , V_{jC} , W_{jC} denote respectively, BiCG matrices and vectors, obtained by applying QMR/BiCG to $Ax = b$ and to $Cx = c$ where $c = U^H b$, $r_{0C} = U^H r_{0A}$ and $\tilde{r}_{0C} = U^T \tilde{r}_{0A}$. Then for each j , $T_{jA} = T_{jC}$, $V_{jA} = U V_{jC}$, and $W_{jA} = \bar{U} W_{jC}$, where \bar{U} is the complex conjugate of U . Furthermore if all of the iterates are well-defined for each method, corresponding iterates and residuals satisfy

$$x_{jA}^{B,Q} = U x_{jC}^{B,Q} \quad \text{and} \quad r_{jA}^{B,Q} = U r_{jC}^{B,Q}. \quad (29)$$

Therefore, for either method, the two corresponding computations yield identical residual and error norms,

$$\|r_{j_A}^{B,Q}\| = \|r_{j_C}^{B,Q}\| \quad \text{and} \quad \|e_{j_A}^{B,Q}\| = \|e_{j_C}^{B,Q}\|. \quad (30)$$

We use theorem 4.1 to construct a set of test matrices where we can vary the nonnormality of the matrix by modifying a simplified eigenvector matrix. The first part of the proof of theorem 4.2 follows from the successive applications of a Jordan decomposition of $A = XJX^{-1}$, a singular value decomposition of X , and theorem 4.1. The second part of the theorem follows from the fact that complex eigenvalues of a real matrix must occur in complex conjugate pairs with corresponding eigenvectors which are complex conjugates of each other. For details see [10].

Theorem 4.2 (Exact arithmetic). For either GMRES, FOM, QMR, or BiCG, all possible residual norm plots and all possible error norm plots generated by an application of the method to $Ax = b$ can be generated using arbitrary right-hand sides and matrices of the form

$$C = \Sigma C_N \Sigma^{-1} \quad \text{where } C_N = V^H J V, \quad (31)$$

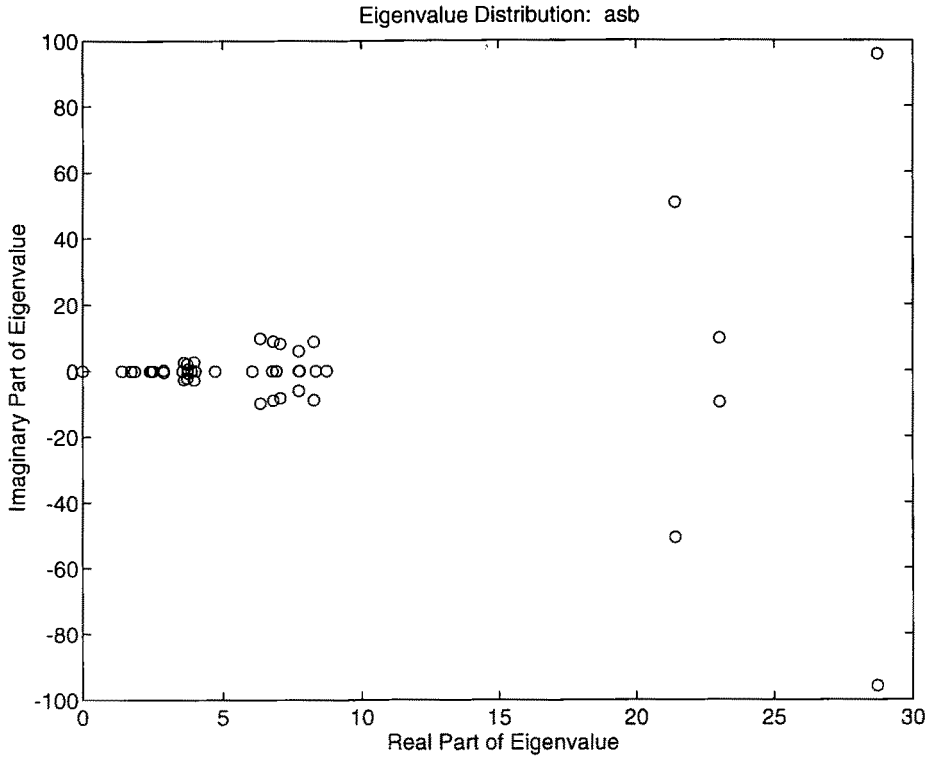
Σ is a diagonal matrix with positive diagonal entries, V is a unitary matrix and J is a Jordan canonical form. For diagonalizable matrices, J is a diagonal matrix Λ of eigenvalues, and C_N is a normal matrix. For real and diagonalizable matrices, we can use a real orthogonal matrix V and a real block diagonal matrix Λ with 1×1 and 2×2 blocks.

Therefore, to study the behavior of any of these Krylov subspace methods on diagonalizable matrices it is sufficient to consider matrices with eigenvector matrices of the form ΣV^H where Σ is a positive diagonal matrix and V is a unitary matrix. We can use equations (31) to specify various eigenvalue distributions and modify the nonnormality of the matrix by modifying Σ and V . In the numerical experiments discussed in section 5 we used the real form in theorem 4.2.

4.4. How should we define b or x_{true} ?

If we wish to compare the behavior of these methods on a given test problem, we may select any vector for x_{true} or b . However, if we wish to compare differences in behavior across a set of test problems, then we must choose these vectors more carefully. In our first set of experiments we not only want to compare the convergence behavior of QMR and GMRES but we also want to compare the convergence behavior of each method across changes in the nonnormality of A . In our second set of experiments we want to compare the convergence behavior of QMR across changes in the eigenvalue distribution of A .

Since we used the real form in theorem 4.2, columns of $X \equiv \Sigma V^H$ corresponding to complex eigenvalues of A were not eigenvectors of A . For each test matrix we scaled the columns of X so that $AX_s = X_s \Lambda$ and corresponding eigenvectors of A obtained from the scaled X_s had unit norm.

Figure 1. Eigenvalue distribution: Λ_{asb} .

In each figure, figures 2–9, we fixed the eigenvalue distribution and the matrix V , and varied the nonnormality of the test matrix by varying the matrix Σ . For each of those tests, we generated a random vector γ and set $b = X_s \Lambda \gamma$. This choice preserves the sizes of the projections of b on the unit right eigenvectors of each test matrix and allows us to make comparisons across the test matrices.

In figures 10–11 we fixed the nonnormality, as defined by Σ and V , and varied the eigenvalue distribution. For each of these tests, we generated a random vector γ and set $b = X_s \gamma$. See [10] for more details.

The test matrices defined by theorem 4.2 are invariant under any scaling of the Σ matrices. We scaled each Σ matrix by $1/\sqrt{\sigma_1 \sigma_n}$ so that the scaled singular values and the inverses of the scaled singular values were in the same interval.

4.5. What software implementations of GMRES and QMR should we use?

We used the MATLAB Templates [1]. We constructed additional MATLAB codes which allow the user to generate test matrices of the form given in equation (31), to call MATLAB Template codes for solving equation (1), and to plot the output. In the Templates codes, estimates of the norms of the residuals are obtained recursively and used to track convergence. However, in each of our tests, we also computed the true residual norms and the true error norms, and we used the true residual norms to

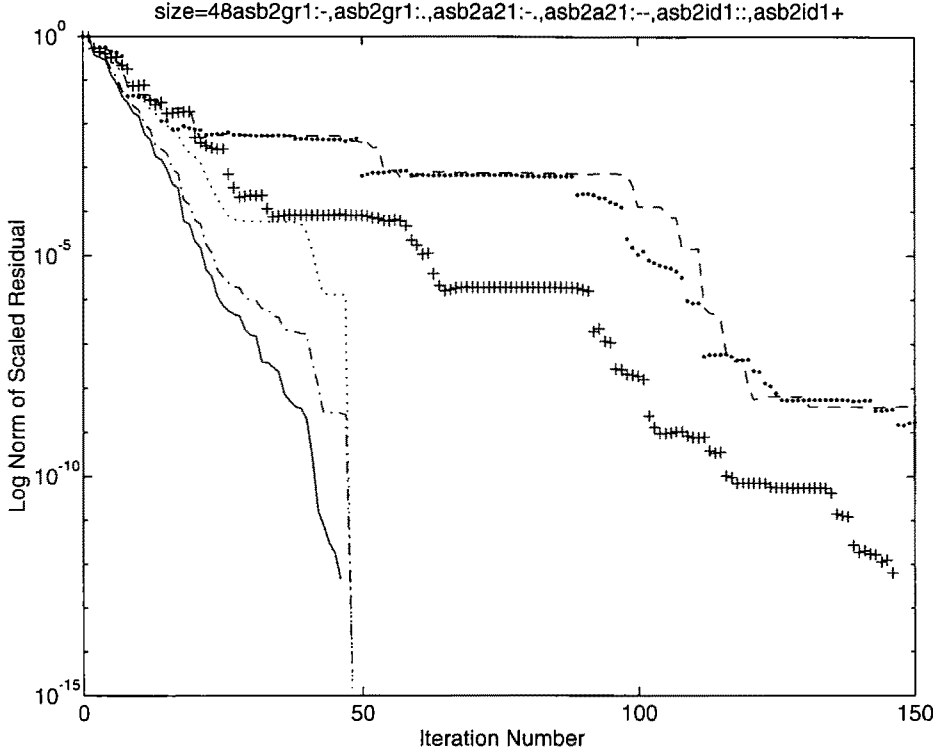


Figure 2. Residual norms versus iteration number: comparisons of GMRES versus QMR residual norms, and of variations of residual norms with increasing nonnormality of the test matrices: three test matrices: asb2gr, asb2a2, and asb2id: eigenvalue distribution; Λ_{asb} which contains complex and real eigenvalues and has large and small complex outliers: corresponding singular value distributions; gr $\equiv \Sigma_s$, a2 $\equiv \Sigma_a$, and id $\equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

track the convergence. In figures 2, 4, 6, 8 and 10, we plotted the true residual norms scaled by the norm of the starting residual. We note also that in QMR and BiCG in [1], $v_1 = w_1 = \tilde{r}_0 = r_0$.

5. Numerical experiments and observations

5.1. Test problems used

All test problems were real matrices of size $n = 48$ and of the real form given in theorem 4.2. We generated an orthogonal matrix V_R using the MATLAB functions RAND and ORTH. We constructed and used three Σ matrices, Σ_I , Σ_s and Σ_a . Σ_I is the identity matrix and was used to generate normal test problems. Σ_a was generated by computing the 48 points in the interval $[10^{-4}, 1]$ whose logarithms of their square roots are equally spaced in the interval $[10^{-2}, 1]$, and applying the scaling $1/\sqrt{\sigma_1\sigma_n}$ to those values. Σ_s was obtained from the Grcar matrix of size 48 [28] by applying the

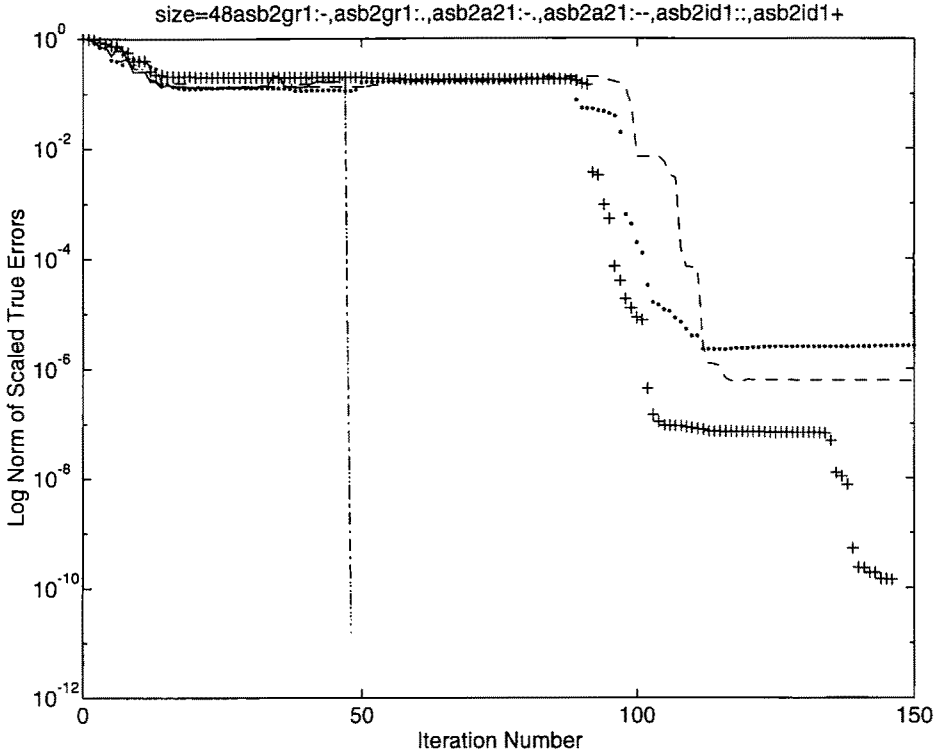


Figure 3. Error norms versus iteration number corresponding to figure 2: comparisons of GMRES versus QMR error norms, and of variations of error norms with increasing nonnormality of the test matrices: three test matrices: asb2gr, asb2a2, and asb2id: eigenvalue distribution; Λ_{asb} which contains complex and real eigenvalues and has large and small complex outliers: corresponding singular value distributions; $\text{gr} \equiv \Sigma_s$, $\text{a2} \equiv \Sigma_a$, and $\text{id} \equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

MATLAB function EIG to this matrix, applying the MATLAB function SVD to the computed right eigenvector matrix X_G to obtain a singular value decomposition $X_G = U_{X_G} \Sigma_{X_G} V_{X_G}^H$, and then scaling the computed singular values. The computed singular values of Σ_{X_G} vary from 5.3×10^{-8} to 4.5. [22] contains results of experiments on iterative methods applied to the Gcar matrix.

We constructed 10 eigenvalue distributions by modifications of the eigenvalue distribution Λ_{asb} depicted in figure 1. Λ_{asb} has two small pairs of complex outliers with magnitudes 10^{-2} and 10^{-4} , has three large pairs of complex outliers with magnitudes 25, 55 and 100, and the other eigenvalues were generated randomly as real or complex in the box $[1, 10] \times [-10, 10]$. The other eigenvalue distributions were obtained from Λ_{asb} by systematically modifying the outliers, both small and large, and by changing the outliers and the other eigenvalues from complex to nearly real. These distributions are summarized in table 1. N-Real means nearly-real, and is obtained by multiplying the imaginary parts of the eigenvalues by 10^{-12} . Similarly, N-Imag means nearly-purely-imaginary. Mixed means there are both complex and real eigenvalues. All of the eigenvalues have positive real parts.

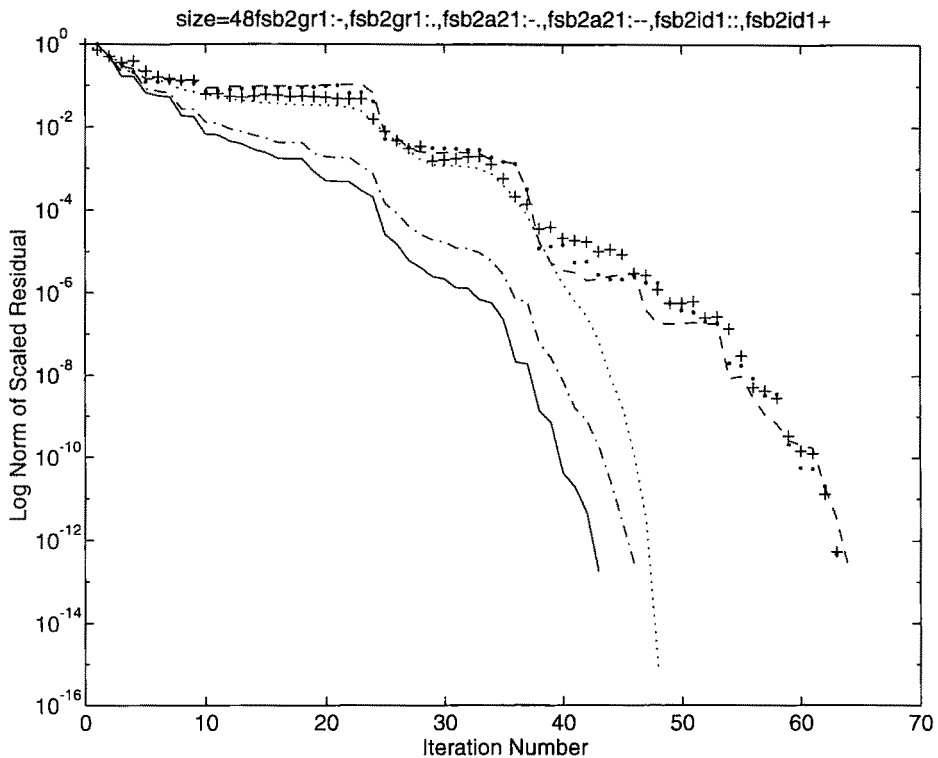


Figure 4. Residual norms versus iteration number: comparisons of GMRES versus QMR residual norms, and of variations of residual norms with increasing nonnormality of the test matrices: three test matrices: fsb2gr, fsb2a2, and fsb2id: eigenvalue distribution; Λ_{fsb} which contains complex and real eigenvalues but does not have any outliers: corresponding singular value distributions; gr $\equiv \Sigma_s$, a2 $\equiv \Sigma_a$, and id $\equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

Table 1
Eigenvalue distributions which were used in figures 1–11.

Eigenvalue distribution	Type	Small outliers magnitudes	Type	Large outliers magnitudes	Type
Λ_{ash}	Mixed	$10^{-4}, 10^{-2}$	Complex	25, 55, 100	Complex
Λ_{hsh}	Mixed	.96, 10^{-2}	Complex	25, 55, 100	Complex
Λ_{dsh}	Mixed	.96, .99	N-Imag	25, 55, 100	Complex
Λ_{esh}	Mixed	$10^{-4}, 10^{-2}$	Complex	None	
Λ_{fsh}	Mixed	.96, .99	N-Imag	None	
Λ_{msb}	Mixed	$10^{-4}, 10^{-2}$	N-Real	25, 55, 100	Complex
Λ_{nsh}	Mixed	$10^{-4}, 10^{-2}$	N-Real	25, 55, 100	N-Real
Λ_{osh}	N-Real	$10^{-4}, 10^{-2}$	N-Real	21, 23, 28	N-Real
Λ_{psh}	N-Real	.96, .99	N-Real	21, 23, 28	N-Real
Λ_{qsb}	N-Real	.26, .265	N-Real	None	

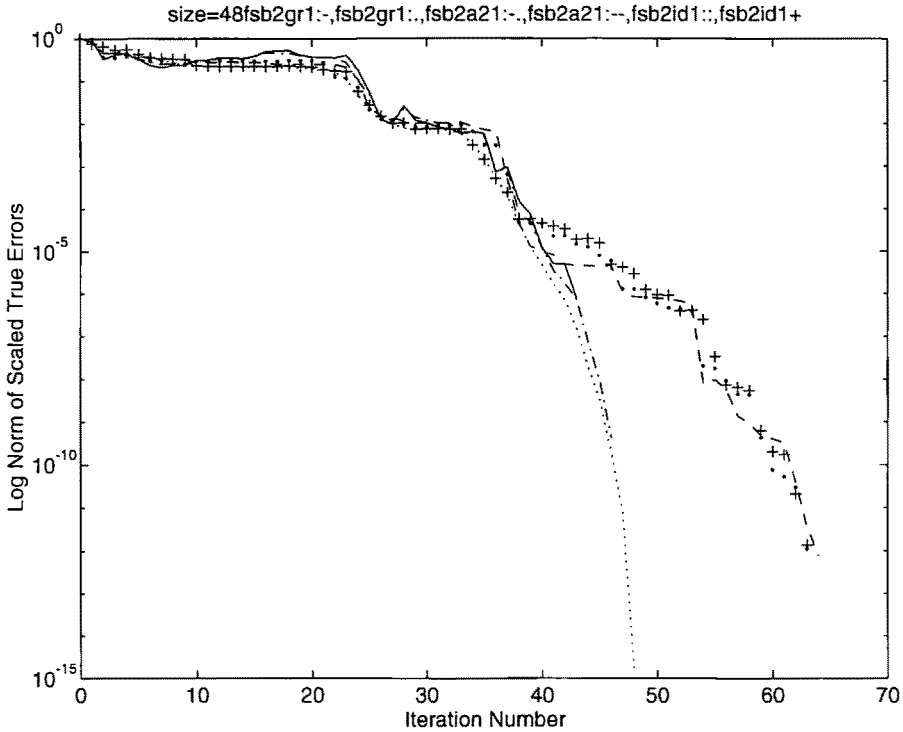


Figure 5. Error norms versus iteration number corresponding to figure 4: comparisons of GMRES versus QMR error norms, and of variations of error norms with increasing nonnormality of the test matrices: three test matrices: fsb2gr, fsb2a2, and fsb2id: eigenvalue distribution; Λ_{fsb} which contains complex and real eigenvalues but does not have any outliers: corresponding singular value distributions; $gr \equiv \Sigma_s$, $a2 \equiv \Sigma_a$, and $id \equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

Table 2

Real test matrices: theorem 4.2. $A = X\Lambda_A X^{-1}$ with X real and Λ real and block diagonal. $X \equiv U_X \Sigma_X V_X^H$, $U_X^H U_X = V_X^H V_X = I$, and eigenvalues defined by 1×1 or 2×2 blocks in Λ_A .

Test matrix A	Λ_A	U_X	Σ_X	V_X
asb2gr	Λ_{usb}	I	Σ_s	V_R
asb2a2	Λ_{usb}	I	Σ_a	V_R
asb2id	Λ_{usb}	I	Σ_I	V_R

We then used Σ_I , Σ_s , Σ_a , V_R , and the different eigenvalue distributions to generate test matrices. Examples of these test matrices are given in table 2. The matrix asb2id is a normal matrix. asb2a2 and asb2gr are nonnormal matrices with asb2a2 constructed to have nonnormality between that of asb2id and asb2gr. The other test matrices were constructed in a similar way using the particular Λ and Σ specified in the caption on each of the figures.

In [11] we observed that small but nonzero entries in strategic positions in V may affect the convergence of eigenvalue computations based upon either the Arnoldi

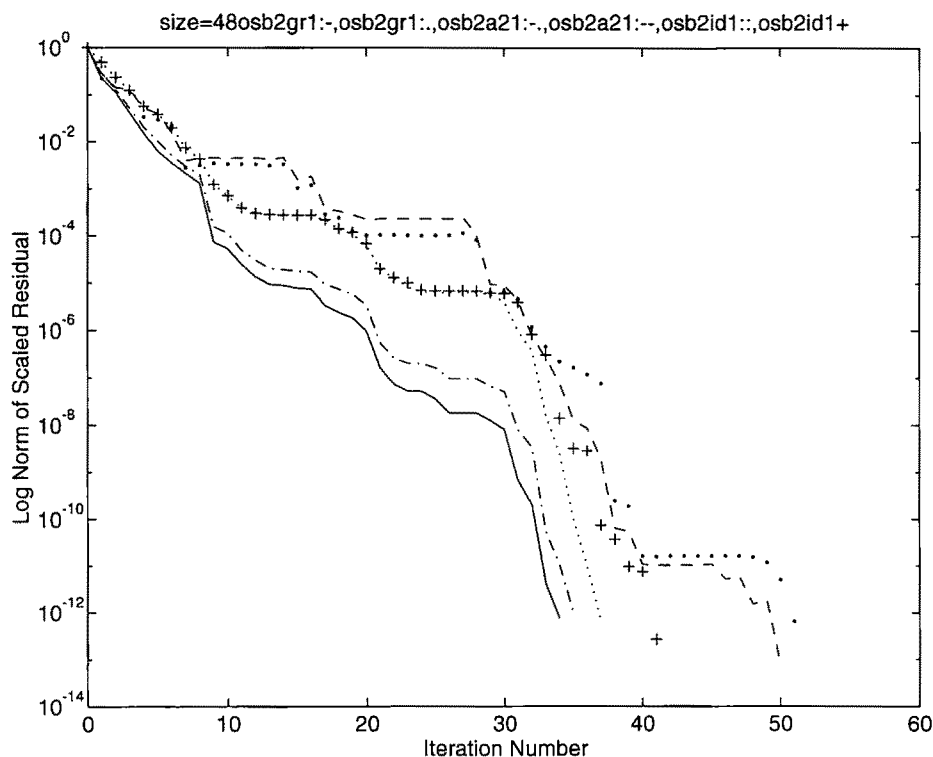


Figure 6. Residual norms versus iteration number: comparisons of GMRES versus QMR residual norms, and of variations of residual norms with increasing nonnormality of the test matrices: three test matrices: osb2gr, osb2a2, and osb2id: eigenvalue distribution; Λ_{osb} nearly real eigenvalues with large and small outliers: corresponding singular value distributions; gr $\equiv \Sigma_s$, a2 $\equiv \Sigma_a$, and id $\equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

or nonsymmetric Lanczos recursions. If V has a nefarious structure which correlates with small outliers, we might expect similar effects upon the convergence of the QMR/GMRES procedures for $Ax = b$. We do not, however, consider such effects in this paper. Also we do not use any form of preconditioning. We include only representative samples of the results of the numerical experiments. See [10] for additional figures.

5.2. Effects of nonnormality on convergence

We compared the observed behavior of QMR and GMRES across several problems with variations in Σ in attempts to determine the sensitivity of these methods to increasing nonnormality. We present the results of four of these tests which are indicative of the overall test results. See figures 2–9. In each of these figures the eigenvalue distribution is fixed and we plotted the scaled GMRES and QMR residual or error norms generated by the application of each method to each of the three

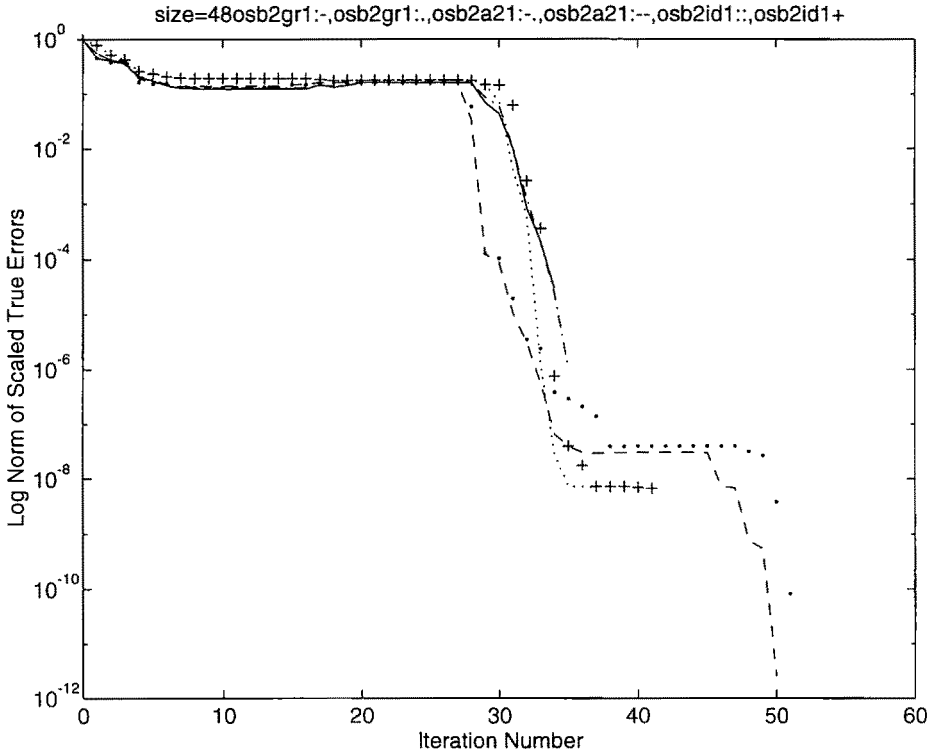


Figure 7. Error norms versus iteration number corresponding to figure 6: comparisons of GMRES versus QMR error norms, and of variations of error norms with increasing nonnormality of the test matrices: three test matrices: osb2gr, osb2a2, and osb2id: eigenvalue distribution; Λ_{osb} which real eigenvalues with large and small outliers: corresponding singular value distributions; gr $\equiv \Sigma_s$, a2 $\equiv \Sigma_a$, and id $\equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

test problems corresponding to the specified eigenvalue distribution and the three Σ matrices, Σ_I , Σ_a and Σ_s .

Figures 2 and 3 correspond to the eigenvalue distribution Λ_{asb} which has both complex and real eigenvalues and both large and small complex pairs of outliers. Figures 4 and 5 correspond to Λ_{fsb} which has complex and real eigenvalues but no small or large outliers. Figures 6 and 7 correspond to Λ_{osb} which has nearly real eigenvalues and both large and small outliers. Figures 8 and 9 correspond to Λ_{qsb} which has nearly real eigenvalues and no outliers.

We observe, see figures 2, 4, 6 and 8, that the GMRES residual norms decreased significantly more rapidly than the corresponding QMR residual norms. However, see figures 3, 5, 7 and 9, we do not observe corresponding differences in the GMRES and QMR error norm plots. In fact, in each of these figures, the initial portions of the QMR and of the GMRES error norm plots are very similar across the changes in nonnormality which we considered. The rapid decreases in the GMRES residual norms lead to premature termination of those computations on several test problems.

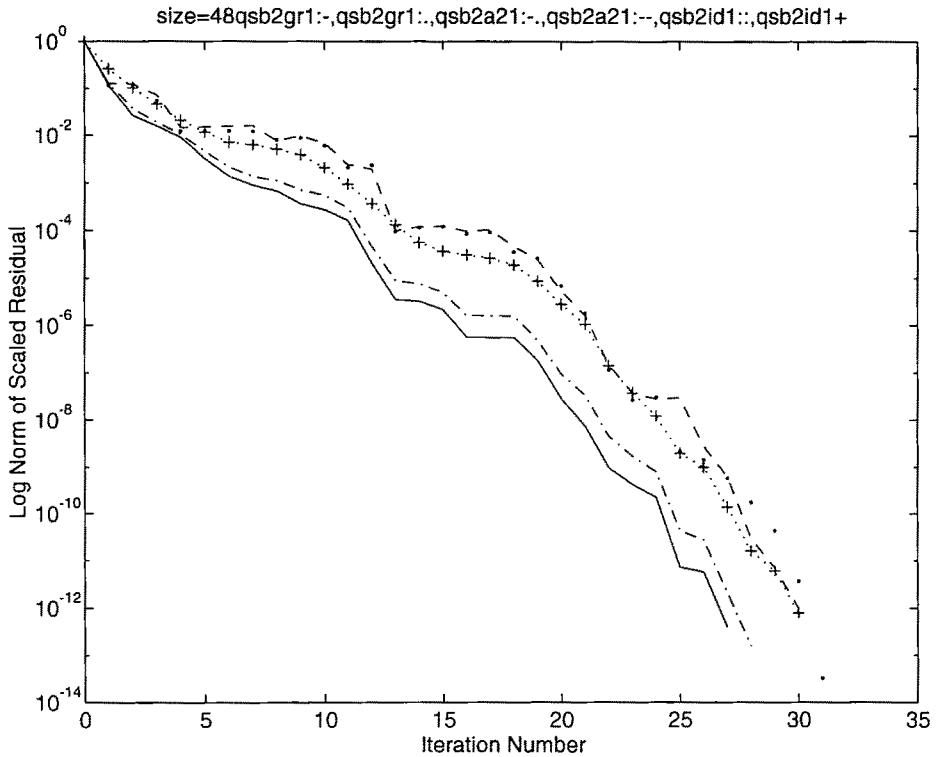


Figure 8. Residual norms versus iteration number: comparisons of GMRES versus QMR residual norms, and of variations of residual norms with increasing nonnormality of the test matrices: three test matrices: qsb2gr, qsb2a2, and qsb2id: eigenvalue distribution; Λ_{qsb} nearly real eigenvalues with no outliers: corresponding singular value distributions; gr $\equiv \Sigma_s$, a2 $\equiv \Sigma_a$, and id $\equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

In each of the figures, figures 2, 4, 6 and 8, we also observe that the GMRES residual norms decreased as we increased the nonnormality of the test matrix as specified by the choice of Σ . The GMRES residual norm curve corresponding to the normal problems is an upper envelope for the GMRES residual norm curves corresponding to the nonnormal problems.

If we consider the corresponding QMR residual norm curves we observe in figures 2, 4, 6 and 8 that the residual norms corresponding to the nonnormal problems are fairly close together. Moreover, on all of the test problems, the QMR residual norm curves appear to provide a more realistic estimate of the behavior of the corresponding error norm curves than the GMRES residual norms do.

When the eigenvalues are nearly real, see figures 6 and 8, the GMRES and the QMR residual norm plots for the normal problems track each other, at least initially, as they should. The effects of outliers on the GMRES convergence can only be seen in the error norm plots, figures 3 and 7. Whenever small outliers are present, all of the significant error reductions in the GMRES error norms occurred on the last few iterations.

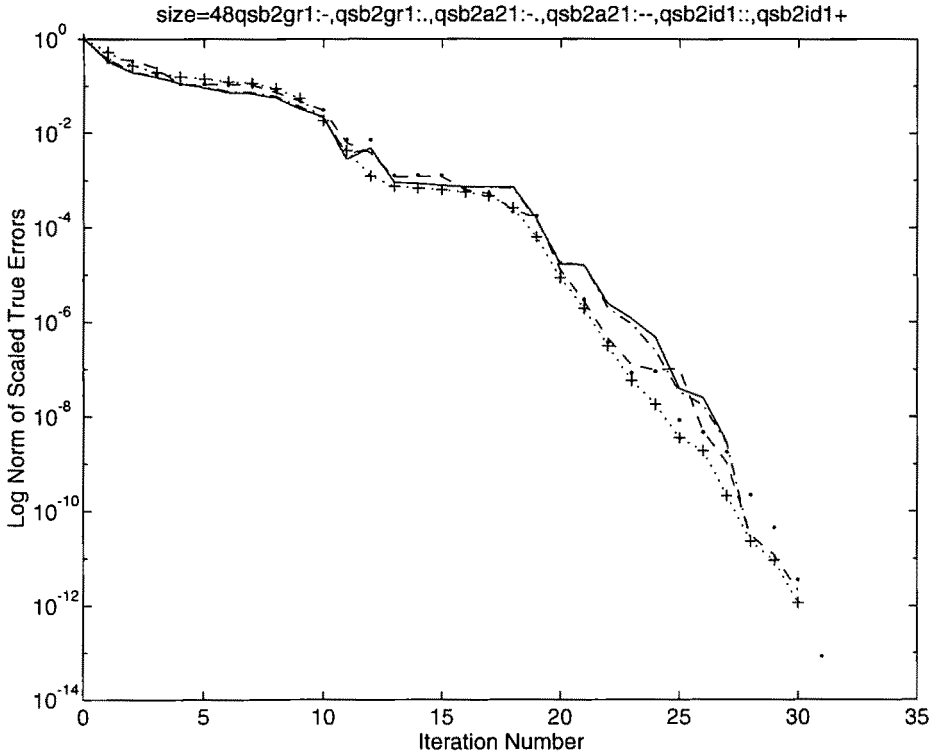


Figure 9. Error norms versus iteration number corresponding to figure 8: comparisons of GMRES versus QMR error norms, and of variations of error norms with increasing nonnormality of the test matrices: three test matrices: qsb2gr, qsb2a2, and qsb2id: eigenvalue distribution; Λ_{qsb} nearly real eigenvalues with no outliers: corresponding singular value distributions; gr $\equiv \Sigma_s$, a2 $\equiv \Sigma_a$, and id $\equiv \Sigma_I$. Symbols for GMRES residual norms: solid (gr), dot-dash (a2), small dots (id). Symbols for QMR residual norms: big dots (gr), dashes (a2), + (id).

We note that in each of these tests the estimates of the GMRES residual norms and the estimates of the QMR residual norms were good approximations to the true residual norms.

5.3. Outliers and their effect on the convergence of QMR

In the first set of experiments we observed significant changes in the number of iterations required by QMR as we varied the outliers and whether or not the eigenvalues and the outliers were real or complex. The number of QMR iterations required appeared to be more sensitive to changes in outliers than to the changes in nonnormality which we used. However, our choice of b in those experiments did not allow us to make comparisons across different eigenvalue distributions. In order to make such comparisons, we ran a second set of experiments where we fixed the matrix X_s as defined in section 4.4, varied the block eigenvalue matrix Λ , and set $b \equiv X_s \gamma$. This choice fixes the sizes of the projections of b on each unit right eigenvector of each test matrix as we vary the eigenvalue distribution but can correspond to distorted x_{true} . We

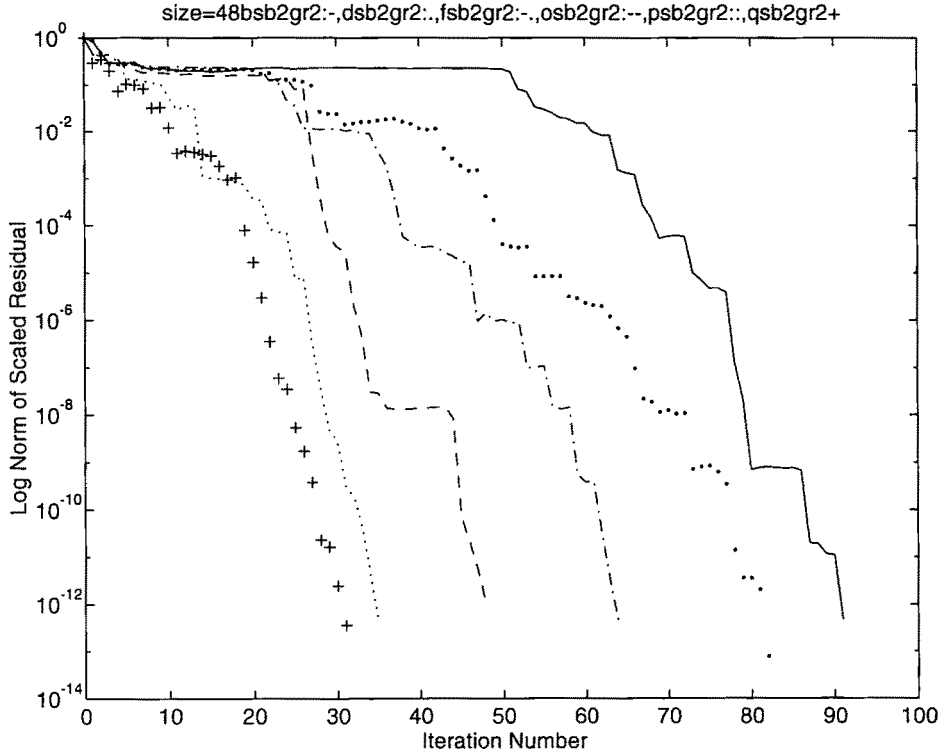


Figure 10. QMR residual norms versus iteration number: fixed nonnormality; singular value distribution: $gr \equiv \Sigma_s$; comparison of QMR residual norm convergence as we modify the eigenvalue distribution. Eigenvalue distributions: solid (Λ_{hsb2} , complex and real eigenvalues with complex pairs of outliers with magnitudes 10^{-2} , 25, 55 and 100; big dots (Λ_{dsb2} , complex and real eigenvalues with complex pairs of outliers with magnitudes 25, 55 and 100); dot-dash (Λ_{fsb2} , complex and real eigenvalues with no outliers); dash-dash (Λ_{osh2} , nearly-real eigenvalues with outliers with magnitudes 10^{-2} , 10^{-4} , 21, 23 and 28); small dots (Λ_{psb2} , nearly-real eigenvalues with outliers with magnitudes 21, 23, and 28); + (Λ_{qsb2} , nearly-real eigenvalues with no outliers).

present the results of tests across one subset of eigenvalue distributions. See figures 10 and 11. See [10] for the results of additional tests.

We considered the eigenvalue distributions

$$\Lambda_{bsb}, \Lambda_{dsb}, \Lambda_{fsb}, \Lambda_{osb}, \Lambda_{psb} \quad \text{and} \quad \Lambda_{qsb}. \quad (32)$$

Using table 1, we observe that with this choice of eigenvalue distributions, we move from a distribution with mixed eigenvalues, a small complex pair of outliers and three large complex pairs of outliers systematically to a distribution of nearly real eigenvalues with no outliers. We present only the results for the nonnormal test problems corresponding to Σ_s . The results for the corresponding normal problems Σ_I were very similar.

Figure 10 clearly illustrates the significant decreases in the numbers of iterations required for residual norm convergence achieved by systematically simplifying the

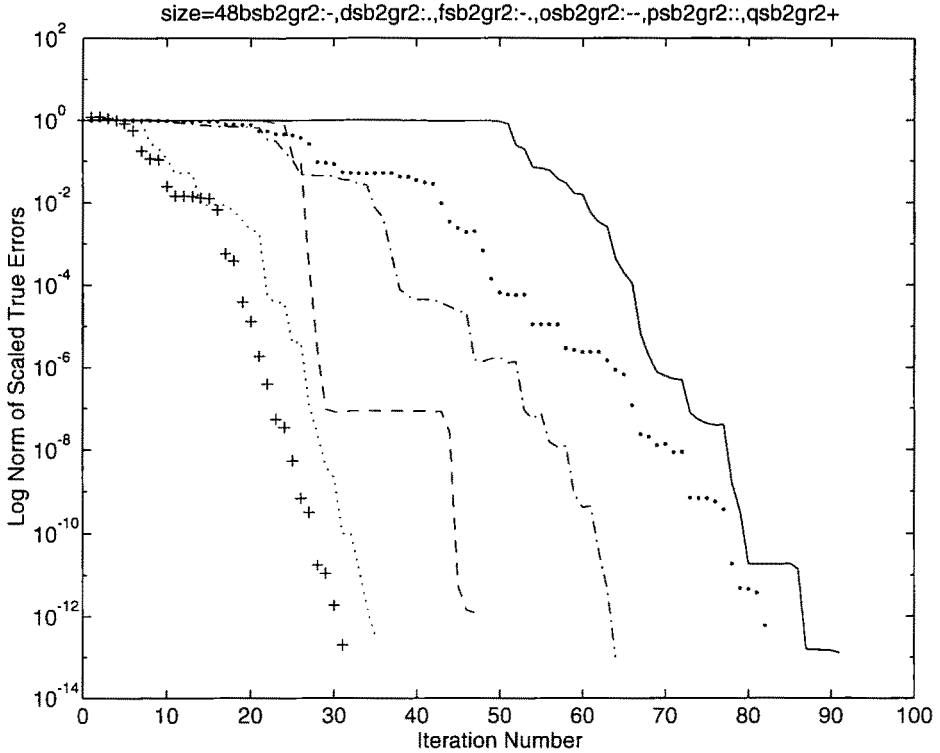


Figure 11. QMR error norms versus iteration number corresponding to figure 10: fixed nonnormality; singular value distribution: $gr \equiv \Sigma_s$; comparison of QMR error norm convergence as we modify the eigenvalue distribution. Eigenvalue distributions: solid (Λ_{hsh2} , complex and real eigenvalues with complex pairs of outliers with magnitudes 10^{-2} , 25, 55 and 100; big dots (Λ_{dsh2} , complex and real eigenvalues with complex pairs of outliers with magnitudes 25, 55 and 100); dot-dash (Λ_{fsh2} , complex and real eigenvalues with no outliers); dash-dash (Λ_{osh2} , nearly-real eigenvalues with outliers with magnitudes 10^{-2} , 10^{-4} , 21, 23 and 28); small dots (Λ_{psh2} , nearly-real eigenvalues with outliers with magnitudes 21, 23, and 28); + (Λ_{qsh2} , nearly-real eigenvalues with no outliers).

eigenvalue distribution. These reductions occur independently of the nonnormality of the test matrices. See [10]. In figure 11 we observe that at least for these test problems, the corresponding error norm plots track the residual norms.

6. Summary

We derived a relationship between residual norms generated by the BiCG method and residual norms generated by the FOM method. This relationship states that any residual norm plots seen in a BiCG computation can also be seen in a FOM computation on a different problem but with the same eigenvalues. In this global sense, these two types of procedures are identical. In practice, however, we are interested in how these procedures behave when they are applied to the same matrix problems.

Therefore, we ran two sets of numerical experiments using test matrices where we could systematically modify the nonnormality of the test matrices by modifications

on simplified eigenvector matrices. We compared the behavior of each method as a function of the nonnormality of the test matrix.

We observed that changes in nonnormality may produce unexpected effects upon the GMRES residual norm convergence, providing misleading indications of superior convergence over QMR when the GMRES error norms are not significantly different from those for QMR. This behavior could lead to premature termination of the GMRES procedure.

For the changes in nonnormality which we considered we observed that the convergence of the QMR residual and error norms was primarily controlled by the presence or absence of outliers and by the character, real or complex, of these and the other eigenvalues. For GMRES the effects of changes in the eigenvalue distribution are exhibited clearly only in the corresponding GMRES error norm plots.

In [11] we considered similar questions for the eigenvalue problem $Ax = \lambda x$.

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