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ERROR ANALYSIS OF KRYLOV METHODS IN A NUTSHELL*

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Abstract. Error and residual bounds for the matrix iteration methods BiCG, QMR, FOM, and GMRES are derived in a simple and unified way.

Key words. Krylov subspace methods, conjugate–gradient-type methods, Arnoldi method, Lanczos method, error bounds

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1. Introduction. In this short note we present error bounds for iterative methods for the solution of linear systems

$$Ax = b,$$

where A is a nonsingular complex matrix of (large) dimension N and $b \in \mathbf{C}^N$ is a given vector. To simplify the presentation we assume throughout that b is of unit length, $\|b\| = 1$ in the Euclidean norm.

In the literature, some residual and error bounds for the most common Krylov subspace methods have been obtained previously [2, 3, 4, 6, 9, 13, 14, 17, 18, 19, 22]. The derivations of these results appear rather unrelated to each other, and the existing results make it difficult to compare the approximation properties of the different methods.

In the present note we derive in a unified and very simple way new error bounds for (look-ahead) BiCG, QMR, FOM, and GMRES. These bounds are all of similar type. They exhibit not only the common underlying polynomial approximation problem but in addition show which factors may cause different behavior of the methods.

2. The methods. Krylov subspace methods yield approximations to $x = A^{-1}b$ of the form

$$x_m = V_m y_m, \qquad V_m \in \mathbf{C}^{N\times m}, \quad y_m \in \mathbf{C}^m, \tag{2.1}$$

where the columns of $V_m = [v_1, \ldots, v_m]$ form a basis of the Krylov space $K_m = \operatorname{span}(b, Ab, \ldots, A^{m-1}b)$.

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We consider two methods of constructing the basis V_m (Arnoldi and Lanczos processes) and two different ways of defining the coefficient vector y_m (Galerkin and (quasi-) minimal-residual approaches).

The *Arnoldi process* [1] generates an orthonormal basis V_m and a Hessenberg matrix $\widetilde{H}_m$ of dimension $(m+1) \times m$ (which is the upper left part of its successor $\widetilde{H}_{m+1}$) such that

$$AV_m = V_{m+1}\tilde{H}_m. \tag{2.2}$$

Due to the orthogonality of V_{m+1} we have

$$V_{m+1}^* A V_m = \widetilde{H}_m \quad \text{and} \quad V_m^* A V_m = H_m,$$

where H_m is the upper square block of $\widetilde{H}_m$, i.e., $H_m = [I_m 0]\widetilde{H}_m$.

The *look-ahead Lanczos process* [11, 20, 8] works with short recurrences for the construction of the Krylov basis. Here, one computes in addition to a basis V_m of K_m an auxiliary basis $W_m = [w_1, \ldots, w_m]$ which spans the Krylov subspace with respect to A^* and w_1. The Lanczos vectors v_j and w_j are constructed such that they satisfy a biorthogonality condition, or block biorthogonality in case of the look-ahead version, i.e., $D_m := W_m^* V_m$ is block diagonal. The look-ahead process ensures that D_m is well conditioned when the index m terminates a block. As for the Arnoldi method, one obtains a matrix representation (2.2) but now with a block tridiagonal matrix $\widetilde{H}_m$ (still Hessenberg) satisfying

$$W_{m+1}^* A V_m = D_{m+1}\widetilde{H}_m \quad \text{and} \quad W_m^* A V_m = D_m H_m. \tag{2.3}$$

However, unlike the Arnoldi case, neither V_m nor W_m are orthogonal matrices. It is usual to scale the Lanczos vectors to have unit norm, in which case the norms of V_m and W_m are bounded by $\sqrt{m}$.

We note that the matrix relations for the Arnoldi process are formally the same as for the Lanczos process when we set $W_m = V_m$ and $D_m = I_m$.

The definition of the coefficient vector y_m in (2.1) is based on the residual vector

$$r_m = b - Ax_m = V_{m+1}(e_1 - \widetilde{H}_m y_m). \tag{2.4}$$

Here, e_1 is the first unit vector. The Galerkin approach requires r_m to be orthogonal to the subspace spanned by W_m, i.e., $W_m^* r_m = 0$, which is equivalent to

$$H_m y_m = e_1 \tag{2.5}$$

when m terminates a block. This clearly requires H_m to be nonsingular. Instead of using the Galerkin approach, one can minimize the Euclidean norm of the coefficient vector in (2.4) [9, 18], which yields

$$y_m = \widetilde{H}_m^+ e_1, \qquad \text{with} \quad \widetilde{H}_m^+ = (\widetilde{H}_m^* \widetilde{H}_m)^{-1}\widetilde{H}_m^*. \tag{2.6}$$

If V_m is constructed by the Arnoldi process, then (2.6) corresponds to a minimization of $\|r_m\|$, and in the Lanczos case it corresponds to a quasi minimization. In both cases, iterates are well defined for every index m.

We thus consider four methods whose commonly used acronyms are given in the following table.

	Galerkin	Minimization
Arnoldi	FOM	GMRES
Lanczos	BiCG	QMR

BiCG was introduced by Lanczos [12], FOM was introduced by Saad [17], GMRES was introduced by Saad and Schultz [18], and QMR was introduced by Freund and Nachtigal [9]. See [7] for an overview and further references.

3. Error bounds. The first result concerns the Galerkin-type methods.

THEOREM 1. *If A, H_m, and D_m are nonsingular, then the error of the mth BiCG iterate satisfies*

$$\|A^{-1}b - V_m H_m^{-1} e_1\| \le \|A^{-1}P_m\| \min_{p_m(0)=1} \|p_m(A)b\|,$$

with the projection $P_m = I_N - V_{m+1}\widetilde{H}_m H_m^{-1} D_m^{-1} W_m^*$. The minimum is taken over all polynomials p_m of degree at most m with $p_m(0) = 1$.

For FOM, the same error bound holds with $W_m = V_m$ and $D_m = I_m$.

Proof. By (2.2) and (2.3) we have

$$P_m A V_m = 0.$$

Using $e_1 = D_m^{-1} W_m^* b$, which is how e_1 appears in (2.5), we obtain with the help of (2.2)

$$A^{-1}b - V_m H_m^{-1} e_1 = A^{-1}P_m b = A^{-1}P_m(b - AV_m z_m) \tag{3.1}$$

for arbitrary $z_m \in \mathbf{C}^m$. We note that $b - AV_m z_m = p_m(A)b$, where p_m is a polynomial of degree $\le m$ with $p_m(0) = 1$. Conversely, for every such polynomial, $p_m(A)b$ is of the above form. Taking norms in (3.1) therefore gives the stated result. ∎

For minimization-type methods a similar argument gives the following result.

THEOREM 2. *If A and D_{m+k} for some $k \ge 1$ are nonsingular, then the error of the mth QMR iterate satisfies*

$$\|A^{-1}b - V_m \widetilde{H}_m^+ e_1\| \le \|A^{-1}P_m\| \min_{p_m(0)=1} \|p_m(A)b\|,$$

with the projection $P_m = I_N - V_{m+1}[\widetilde{H}_m \widetilde{H}_m^+, 0] D_{m+k}^{-1} W_{m+k}^*$. The minimum is taken over all polynomials p_m of degree at most m with $p_m(0) = 1$.

For GMRES, the same error bound holds with $k = 1$, $W_m = V_m$, and $D_m = I_m$, viz., with the orthogonal projection $P_m = I_N - V_{m+1}\widetilde{H}_m \widetilde{H}_m^+ V_{m+1}^*$.

Remark. In contrast to the Galerkin methods, the projection P_m of the minimization methods can be bounded independently of $\widetilde{H}_m$.

Proof. Since by (2.3)

$$D_{m+k}^{-1} W_{m+k}^* A V_m = \widetilde{H}_{m+k-1} \begin{bmatrix} I_m \\ 0 \end{bmatrix} = \begin{bmatrix} \widetilde{H}_m \\ 0 \end{bmatrix},$$

and since $\widetilde{H}_m^+ \widetilde{H}_m = I_m$, we have again $P_m A V_m = 0$. As in the previous proof we obtain

$$A^{-1}b - V_m \widetilde{H}_m^+ e_1 = A^{-1}P_m b = A^{-1}P_m \cdot p_m(A)b \tag{3.2}$$

for every polynomial p_m of degree at most m with $p_m(0) = 1$. ∎

The minimal norm of $p_m(A)b$ can be further estimated using the spectrum or the pseudospectrum [21] of A, or further properties of A [15, 16]. For example, there are the following bounds:

(a) If A is diagonalizable, then clearly

$$\|p_m(A)b\| \leq \kappa_e(A) \max_{\lambda} |p_m(\lambda)|,$$

where the maximum is taken over the eigenvalues of A and $\kappa_e(A)$ is the condition number of the matrix containing the eigenvectors of A.

(b) Let E be a convex closed bounded set in the complex plane, and let ϕ be the conformal mapping from the exterior of E onto the exterior of the unit disk that takes infinity to infinity. If the ϵ-pseudospectrum of A is contained in E and $0 \notin E$, then

$$\min_{p_m(0)=1} \|p_m(A)b\| \leq \tfrac{1}{2}\, \ell/\epsilon \cdot |\phi(0)|^{-m},$$

where ℓ is the length of the boundary curve of E. This is shown in [10] using Faber polynomials like in [5, 15].

4. Comparison of residuals. From (3.1) and (3.2) we note that the residual satisfies

$$r_m = P_m b = P_m p_m(A) b \tag{4.1}$$

for arbitrary polynomials p_m of degree at most m with $p_m(0) = 1$. This formula allows us to bound the residuals of the Lanczos-based methods BiCG and QMR in terms of those of the (more expensive) GMRES method. Inserting in (4.1) the residual polynomial of GMRES, we have

$$r_m = P_m r_m^{\mathrm{GMRES}} = P_m Q_{m+1} s_m^{\mathrm{GMRES}},$$

where s_m^{GMRES} is the coefficient vector of the GMRES residual with respect to the Arnoldi basis $Q_{m+1} = [q_1, \ldots, q_{m+1}]$. We observe that Q_{m+1} is the $N \times (m+1)$ orthogonal matrix of the QR decomposition of the Lanczos basis $V_{m+1} = Q_{m+1} R_{m+1}$. Here and in the following, V_{m+1} and W_{m+1} denote the matrices containing the Lanczos vectors, which are assumed to be scaled to have unit norm, and $\widetilde{H}_m$ is the block tridiagonal Hessenberg matrix resulting from the Lanczos process. Similarly, we also have

$$r_m = P_m r_m^{\mathrm{QMR}} = P_m V_{m+1} s_m^{\mathrm{QMR}},$$

where $s_m^{\mathrm{QMR}} = (I_{m+1} - \widetilde{H}_m \widetilde{H}_m^{+}) e_1$ is the coefficient vector of the mth QMR residual with respect to the Lanczos basis. From (4.1) we also get the following identities for the BiCG residuals.

PROPOSITION 3. *Let H_m and D_m be nonsingular, and let g_m be the solution of the linear system*

$$H_m^* g_m = h_{m+1,m} e_m,$$

where $h_{m+1,m}$ is the $(m+1, m)$ entry of $\widetilde{H}_m$. Then we have

$$r_m^{\mathrm{BiCG}} = -v_{m+1} \cdot g_m^* D_m^{-1} W_m^* \cdot r_{m-1}^{\mathrm{GMRES}} \tag{4.2}$$

and

$$\|r_m^{\mathrm{BiCG}}\| = \|g_m\| \cdot \|s_{m-1}^{\mathrm{QMR}}\| \,. \tag{4.3}$$

Proof. Using $D_m^{-1} W_m^* V_{m+1} = [I_m \; 0]$ and $Q_{m+1} = V_{m+1} R_{m+1}^{-1}$, we get for BiCG

$$\begin{aligned} P_m Q_{m+1} &= V_{m+1} R_{m+1}^{-1} - V_{m+1} \begin{bmatrix} I_m \\ h_{m+1,m} e_m^T H_m^{-1} \end{bmatrix} D_m^{-1} W_m^* Q_{m+1} \\ &= V_{m+1} R_{m+1}^{-1} - V_{m+1} \begin{bmatrix} I_m & 0 \\ 0 & 0 \end{bmatrix} R_{m+1}^{-1} - V_{m+1} \begin{bmatrix} 0 \\ h_{m+1,m} e_m^T H_m^{-1} \end{bmatrix} D_m^{-1} W_m^* Q_{m+1} \\ &= v_{m+1} \left(e_{m+1}^T / r_{m+1,m+1} - g_m^* D_m^{-1} W_m^* Q_{m+1} \right), \end{aligned}$$

where $r_{m+1,m+1}$ is the $(m+1)$st diagonal entry of R_{m+1}. To compare BiCG with GMRES, we now insert in (4.1) the $(m-1)$st residual vector of GMRES instead of the mth one. This gives

$$r_m^{\mathrm{BiCG}} = P_m r_{m-1}^{\mathrm{GMRES}} = P_m Q_m s_{m-1}^{\mathrm{GMRES}} = -v_{m+1} g_m^* D_m^{-1} W_m^* Q_m s_{m-1}^{\mathrm{GMRES}}$$

and hence (4.2).

To show (4.3), we insert in (4.1) the $(m-1)$st residual vector of QMR, which gives

$$r_m^{\mathrm{BiCG}} = -v_{m+1} g_m^* s_{m-1}^{\mathrm{QMR}}.$$

From the definition of s_{m-1}^{QMR} and (2.6) we find that $\widetilde{H}_{m-1}^* s_{m-1}^{\mathrm{QMR}} = 0$. On the other hand, we also clearly have $\widetilde{H}_{m-1}^* g_m = [I_{m-1} \; 0] H_m^* g_m = 0$. Since the null space of $\widetilde{H}_{m-1}^*$ is of dimension one, g_m must be a multiple of s_{m-1}^{QMR}. This proves (4.3). ∎

A different relation between the residual norms of BiCG and QMR is given in [9, Proposition 5.2].

From (4.2) we get the residual bounds

$$\|r_m^{\mathrm{BiCG}}\| \le \|W_m (D_m^*)^{-1} g_m\| \cdot \|r_{m-1}^{\mathrm{GMRES}}\| \le \sqrt{m}\, \|(D_m^*)^{-1} g_m\| \cdot \|r_{m-1}^{\mathrm{GMRES}}\|. \tag{4.4}$$

Let us illustrate these bounds for a two-dimensional discrete convection diffusion problem. The coefficient matrix we used is the 400×400 matrix

$$A = T \otimes I_{20} + I_{20} \otimes T^T \qquad \text{with } \; T = \mathrm{tridiag}(-2, 3, -1).$$

The right-hand side vector b was chosen as a random vector. In Figure 4.1 we plotted the true value of the quotient of the mth BiCG residual norm and the $(m-1)$st GMRES residual norm (dotted line). The dash-dotted line shows the factor in the first inequality in (4.4). These two quotients are usually not accessible computationally. They are plotted here only for comparison. The solid line finally shows the factor in the last inequality in (4.4), which is available at negligible costs. In a number of numerical examples we found that the estimate (4.4) describes the behavior of BiCG versus GMRES qualitatively correctly, although it may be quantitatively pessimistic.

PROPOSITION 4. *Let D_{m+1} be nonsingular, and let u_{m+1} be a vector of unit norm that spans the null space of $\widetilde{H}_m^*$. Then*

$$\|r_m^{\mathrm{QMR}}\| \le (m+1)\, \|(D_{m+1}^*)^{-1} u_{m+1}\| \cdot \|r_m^{\mathrm{GMRES}}\|. \tag{4.5}$$

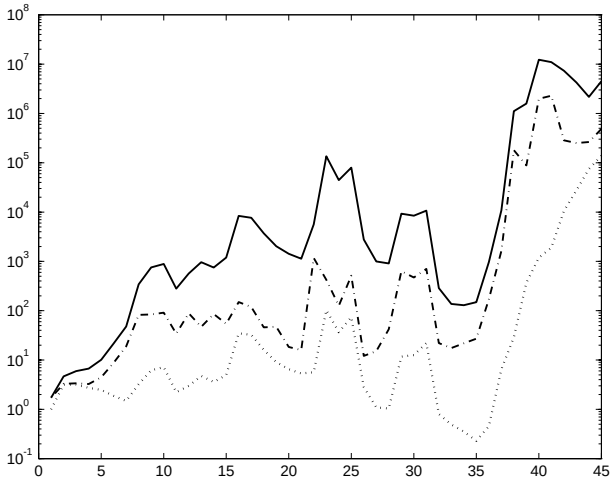

FIG. 4.1. *True and estimated factors between BiCG and GMRES residual norms.*

Proof. If H_{m+1} is invertible, then $u_{m+1} = g_{m+1}/\|g_{m+1}\|$ in the notation of Proposition 3. In this case, the result would follow immediately from Proposition 3. We prefer to give an independent direct proof, which does not require this assumption.

For QMR a similar calculation to that for BiCG gives

$$P_m Q_{m+1} = Q_{m+1} R_{m+1} u_{m+1} u_{m+1}^* R_{m+1}^{-1}. \tag{4.6}$$

Inserting $R_{m+1}^{-1} = D_{m+1}^{-1} W_{m+1}^* Q_{m+1}$ and once more using (4.1) yields (4.5). ∎

Formula (4.6) combined with (4.1) also yields the (computationally inaccessible) residual bound that was previously obtained in [13, section 4.3] with a different argument:

$$\|r_m^{\mathrm{QMR}}\| \le \mathrm{cond}(R_{m+1}) \cdot \|r_m^{\mathrm{GMRES}}\|.$$

The residual of the QMR method applied to $Ax = v_j$ using the Krylov subspaces for the vector b equals $r_m^{(j)} = -V_{m+1} u_{m+1} u_{m+1}^* e_j$. Convergence of QMR implies that, for any fixed j, the jth component of u_{m+1} tends to zero as m becomes large. Therefore, formula (4.5) shows that the influence of early large entries in D_{m+1}^{-1} is damped out as the iteration proceeds. To be more precise, we have by (4.6) and (4.1)

$$r_m^{\mathrm{QMR}} = [r_m^{(1)} \ \cdots \ r_m^{(m+1)}] D_{m+1}^{-1} \cdot W_{m+1}^* r_m^{\mathrm{GMRES}}. \tag{4.7}$$

This explains the success of look-ahead strategies which allow $\|D_{m+1}^{-1}\|$ to become quite large, such as that described in [8].

Similar to Proposition 3, we get for the residuals of FOM and GMRES

$$\|r_m^{\mathrm{FOM}}\| = \|g_m\| \cdot \|r_{m-1}^{\mathrm{GMRES}}\|, \tag{4.8}$$

where g_m is defined as in Proposition 3 but now for the Hessenberg matrix resulting from the Arnoldi process. Note that in the Hermitian case BiCG is equivalent to FOM and, therefore, the first inequality in (4.4) then becomes the equality (4.8).

Further comparisons of the residuals of FOM and GMRES are given in [4].

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REFERENCES

[1] W.E. Arnoldi, *The principle of minimized iterations in the solution of the matrix eigenvalue problem*, Quart. Appl. Math., 9 (1951), pp. 17–29.
[2] R.E. Bank and T.F. Chan, *An analysis of the composite step biconjugate gradient method*, Numer. Math., 66 (1993), pp. 295–319.
[3] T. Barth and T. Manteuffel, *Variable metric conjugate gradient methods*, in Proc. of the 10th International Symposium on Matrix Analysis and Parallel Computing, Keio University, Yokohama, Japan, March 14–16, 1994.
[4] P.N. Brown, *A theoretical comparison of the Arnoldi and GMRES algorithms*, SIAM J. Sci. Statist. Comput., 12 (1991), pp. 58–78.
[5] M. Eiermann, *On semiiterative methods generated by Faber polynomials*, Numer. Math., 56 (1989), pp. 139–156.
[6] S.C. Eisenstat, H.C. Elman, and M.H. Schultz, *Variational iterative methods for nonsymmetric systems of linear equations*, SIAM J. Numer. Anal., 20 (1983), pp. 345–357.
[7] R.W. Freund, G.H. Golub, and N.M. Nachtigal, *Iterative solution of linear systems*, Acta Numerica, 1 (1992), pp. 57–100.
[8] R.W. Freund, M.H. Gutknecht, and N.M. Nachtigal, *An implementation of the look-ahead Lanczos algorithm for non-Hermitian matrices*, SIAM J. Sci. Comput., 14 (1993), pp. 137–158.
[9] R.W. Freund and N.M. Nachtigal, *QMR: A quasi-minimal residual method for non-Hermitian linear systems*, Numer. Math., 60 (1991), pp. 315–339.
[10] M. Hochbruck and Ch. Lubich, *On Krylov subspace approximations to the matrix exponential operator*, SIAM J. Numer. Anal., 1997, to appear.
[11] C. Lanczos, *An iteration method for the solution of the eigenvalue problem of linear differential and integral operators*, J. Res. Natl. Bur. Stand., 45 (1950), pp. 255–282.
[12] C. Lanczos, *Solution of systems of linear equations by minimized iterations*, J. Res. Natl. Bur. Stand., 49 (1952), pp. 33–53.
[13] N.M. Nachtigal, *A Look-ahead Variant of the Lanczos Algorithm and its Application to the Quasi-minimal Residual Method for Non-Hermitian Linear Systems*, Ph.D. dissertation, MIT, Cambridge, MA, 1991.
[14] N.M. Nachtigal, S.C. Reddy, and L.N. Trefethen, *How fast are nonsymmetric matrix iterations?*, SIAM J. Matrix Anal. Appl., 13 (1992), pp. 778–795.
[15] O. Nevanlinna, *Convergence of Iterations for Linear Equations*, Birkhäuser-Verlag, Basel, Switzerland, 1993.
[16] O. Nevanlinna, *Convergence of Krylov–Methods for Sums of Two Operators*, Tech. report A353, Helsinki University of Technology, Helsinki, 1995.
[17] Y. Saad, *Krylov subspace methods for solving large unsymmetric linear systems*, Math. Comp., 37 (1981), pp. 105–126.
[18] Y. Saad and M.H. Schultz, *GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 856–869.
[19] B.A. Schmitt and R. Weiner, *Matrix-free W-methods using a multiple Arnoldi iteration*, Appl. Numer. Math., 18 (1995), pp. 307–320.
[20] D.R. Taylor, *Analysis of the Look-ahead Lanczos Algorithm*, Ph.D. dissertation, University of California at Berkeley, Berkeley, CA, 1982.
[21] L.N. Trefethen, *Pseudospectra of matrices*, Numerical Analysis 1991, D.F. Griffiths and G.A. Watson, eds., Longman Scientific and Technical, Harlow, U.K., 1992, pp. 234–266.
[22] R. Weiss, *Minimization properties and short recurrences for Krylov subspace methods*, Electr. Trans. Numer. Anal., 2 (1994), pp. 57–75.