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SOME REMARKS ON THE ELMAN ESTIMATE FOR GMRES*

B. BECKERMANN†, S. A. GOREINOV‡, AND E. E. TYRTYSHNIKOV‡

Abstract. Starting from a GMRES error estimate proposed by Elman in terms of the ratio of the smallest eigenvalue of the hermitian part and the norm of some nonsymmetric matrix, we propose some asymptotically tighter bound in terms of the same ratio. Here we make use of a recent deep result of Crouzeix and others on the norm of functions of matrices.

Key words. GMRES, nonsymmetric systems, error estimates, field of values

AMS subject classifications. 65F10, 65N22

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1. Introduction.

A popular method for solving nonhermitian systems $Ax = b$ is given by GMRES [13]. Provided that A has a positive definite hermitian part $(A + A^*)/2$, Elman [9] (see also [8]) pointed out the following upper bound for the norm of the kth residual r_k of GMRES for every $k \geq 0$:

$$\frac{\|r_k\|}{\|r_0\|} \leq \sin^k(\beta), \qquad \text{where } \cos(\beta) := \frac{\lambda_{\min}((A + A^*)/2)}{\|A\|} \tag{1.1}$$

with $\beta \in [0, \pi/2)$. Here and hereafter we use $\|\cdot\|$ to denote the Euclidean vector norm or spectral matrix norm. Recall that the field of values (or numerical range)

$$W(A) := \{(Ay, y) : y \in \mathbb{C}^n, \|y\| = 1\}$$

of a matrix is bounded by the rectangle defined by the extremal eigenvalues of the hermitian and the skew-hermitian parts of A. Hence $\lambda_{\min}((A + A^*)/2)$ bounds from below the distance between the origin and $W(A)$. More generally, since $W(A)$ is convex by the Hausdorff theorem, one may show in the case $0 \notin W(A)$ that there is a $t \in \mathbb{R}$ with $\text{dist}(0, W(A)) = \lambda_{\min}((e^{it}A + (e^{it}A)^*)/2)$, and $t \in \{0, \pi\}$ for real matrices A. Since $\|r_k\|$ does not change after multiplying $Ax = b$ by some number of modulus 1, we may rewrite in the case $0 \notin W(A)$ the Elman bound (1.1) as

$$k \geq 0 : \qquad \frac{\|r_k\|}{\|r_0\|} \leq \sin^k(\beta), \qquad \cos(\beta) = \frac{\text{dist}(0, W(A))}{\|A\|}, \tag{1.2}$$

where we recall that (1.2) can be sharper than (1.1).

Estimates (1.1) or (1.2) are obtained by iterating the inequality for $k = 1$ corresponding to a one-dimensional minimization problem, which should allow for some

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†Laboratoire Paul Painlevé UMR 8524 (ANO-EDP), UFR Mathématiques–M3, UST Lille, F-59655 Villeneuve d'Ascq CEDEX, France (bbecker@math.univ-lille1.fr). The research of this author was supported in part by INTAS network NeCCA 03-51-6637, and in part by the Ministry of Science and Technology (MCYT) of Spain and the European Regional Development Fund (ERDF) through grant BFM2001-3878-C02-02.

‡Institute of Numerical Mathematics, Russian Academy of Sciences, Gubkina Street, 8, Moscow, 119991, Russia (serge@inm.ras.ru, tee@inm.ras.ru). The research of these authors was supported in part by RFBR grant 02-01-00590a.

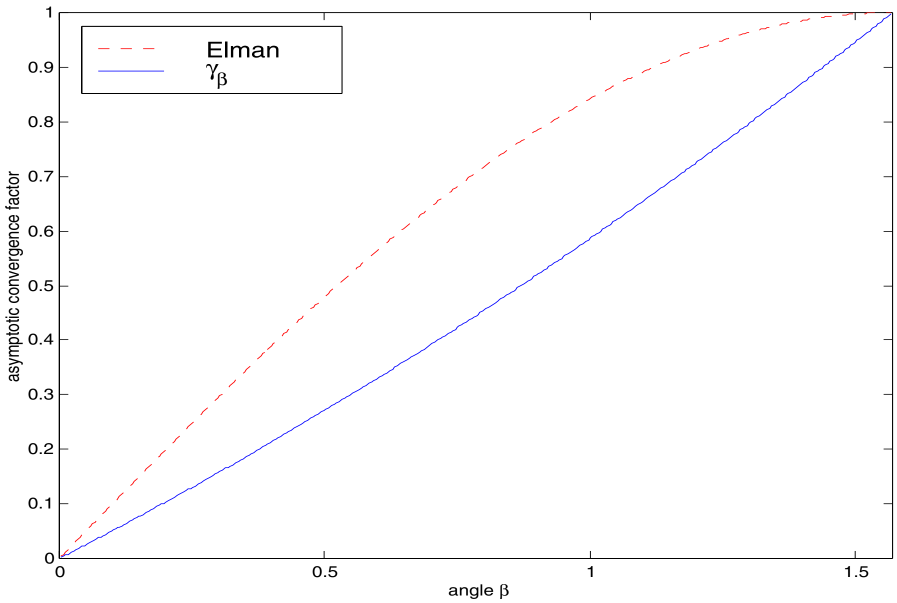

FIG. 1. *Elman's asymptotic convergence factor* $\sin(\beta)$ *(dashed) versus the new asymptotic convergence factor* γ_β *of Theorem* 2.1 *(solid).*

improvements (compare, for instance, the approach in [7, Theorem 6.1] in terms of angles between subspaces). Here we propose some asymptotically sharper bounds only in terms of the above angle $\beta \in (0, \pi/2)$, which to our knowledge seems to be new.

2. Main result.

THEOREM 2.1. *Let A be a matrix with $0 \notin W(A)$, and let $\beta \in (0, \pi/2)$ be as in* (1.2). *Then for the kth relative residual, $k \geq 1$, of GMRES we have*

$$\frac{\|r_k\|}{\|r_0\|} \leq (2 + 2/\sqrt{3})\,(2 + \gamma_\beta)\,\gamma_\beta^k, \tag{2.1}$$

where

$$\gamma_\beta := 2 \sin\left(\frac{\beta}{4 - 2\beta/\pi}\right) < \sin(\beta).$$

All convergence bounds (1.1), (1.2), (2.1) are of the form $C\,\gamma^k$, where we will call C the constant factor and γ the asymptotic convergence factor. We have drawn in Figure 1 the two different asymptotic convergence factors of (1.1) and of Theorem 2.1. Especially for β close to $\pi/2$ (i.e., the critical case where the origin is close to the field of values), the asymptotic convergence factor of Theorem 2.1 is clearly more interesting. However, the constant factor of (2.1) (which can be shown to be not optimum) slightly deteriorates the sharpness of the new convergence bound; see Figure 2. Notice that bounds of type (2.1) do not capture the range of superlinear convergence of GMRES.

Before entering in the proof of Theorem 2.1, let us briefly recall some well-known facts on the convergence of GMRES. Starting from the observation

$$\frac{\|r_k\|}{\|r_0\|} \leq \min\{\|p(A)\| : p \text{ a polynomial of degree} \leq k,\ p(0) = 1\},$$

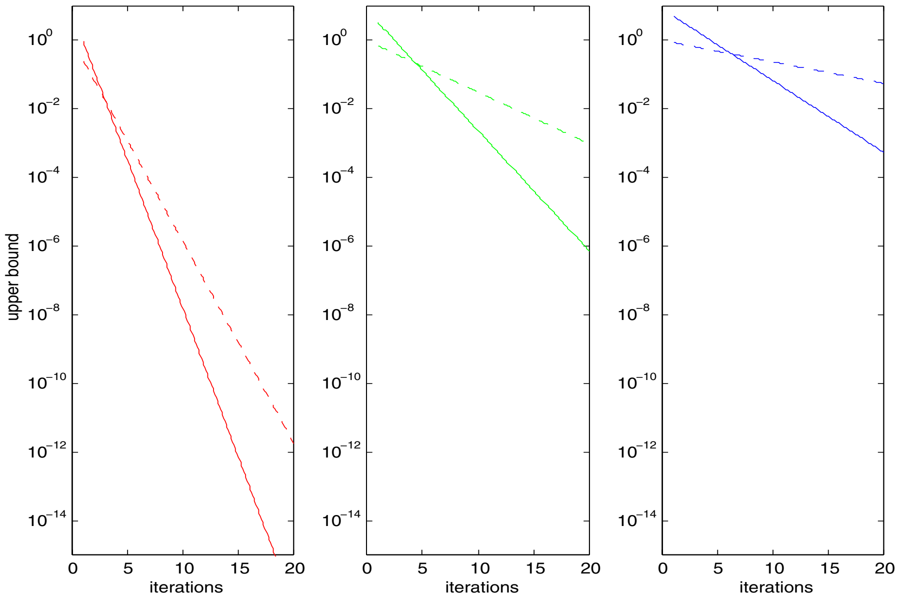

Fig. 2. *Upper bounds for the relative residuals of the kth iterate ($k = 1, \ldots, 20$) of GMRES for $\beta = \pi/12$, $\beta = \pi/4$, $\beta = \pi/3$ (from left to right); the curve corresponding to Elman's bound is dashed, and the one of Theorem* 2.1 *is solid.*

there are many classical GMRES estimates not involving special properties of the right-hand side b of the system; see, for instance, [14, Chapter 6.11] or [10, Chapter 3]. Here the quantity on the right is usually estimated in terms of a polynomial extremal problem: For a compact set K, consider the constrained Chebyshev approximation problem

$$E_k(K) := \min\{\|p\|_K : p \text{ a polynomial of degree} \leq k,\ p(0) = 1\},$$

where by $\|\cdot\|_K$ we denote the maximum norm on K. For instance, for diagonalizable A one immediately obtains the classical bound

$$k \geq 0: \qquad \frac{\|r_k\|}{\|r_0\|} \leq \|V\|\,\|V^{-1}\|\,E_k(\sigma(A)) \tag{2.2}$$

in terms of the spectrum $\sigma(A)$ and the matrix of eigenvectors V of A. Other more sophisticated estimates are based, for instance, on the pseudospectrum, but in general the shape of these sets is difficult to predict. A third group of estimates is obtained via the field of values, starting perhaps with a paper of Eiermann [6]; see also [10]. These estimates are based on the observation that, given a convex set $K \neq \mathbb{C}$, there exists a constant $C(K) < \infty$ such that for all matrices A and for all rational functions f having no pole in K there holds

$$W(A) \subset K \qquad \Longrightarrow \qquad \|f(A)\| \leq C(K)\,\|f\|_K. \tag{2.3}$$

Recently, Crouzeix and his coworkers [1, 3, 4] gave quite deep results concerning (2.3). The existence of such a finite constant in (2.3) depending only on the set K was established by B. Delyon and F. Delyon in [5]. In [1, Corollary 2.3], it was shown that for the optimal constant in (2.3) (also denoted by $C(K)$) one has

$$C(K) \leq 2 + \pi + \int_0^{2\pi} \frac{|\rho'(t)|}{\rho(t)}\, dt, \tag{2.4}$$

where $[0, 2\pi] \ni t \mapsto z_0 + \rho(t)e^{it} \in \partial K,\ \rho(t) > 0$, is any polar parametrization of the boundary of K for some z_0 in the interior of K (the case of a segment K is trivial; here $aI + bA$ is hermitian for some $a, b \in \mathbb{C}$ and thus $C(K) = 1$). The authors also give improved estimates for particular K, e.g., for a sector [4]

$$C(S_\alpha) \leq 2 + 2/\sqrt{3}, \qquad S_\alpha = \{z \in \mathbb{C} : 0 \leq \arg(z) \leq \alpha\}, \quad 0 \leq \alpha \leq \pi. \tag{2.5}$$

In a recent manuscript [3], Crouzeix showed that

$$C(K) \leq 33.75 \tag{2.6}$$

for any convex compact set K, independently of its shape. It is a conjecture of Crouzeix that $C(K)$ in (2.3) can be replaced by the number 2.

Let us return to the proof of Theorem 2.1. By possibly multiplying A with some complex number of modulus 1, we may suppose without loss of generality that the element of $W(A)$ closest to 0 is real positive, and thus

$$W(A) \subset \{z : \mathrm{Re}(z) \geq \|A\| \cos(\beta)\},$$

with β as in (1.2). Define K_β to be the (convex) intersection between the closed unit disk and the half-plane $\{\mathrm{Re}(z) \geq \cos(\beta)\}$. Since $W(A) \subset \{|z| \leq \|A\|\}$, we see that $W(A) \subset \|A\|\, K_\beta$. Moreover, by constructing block-diagonal matrices with blocks

$$B(\phi) = \begin{bmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{bmatrix}, \qquad 0 \leq \phi \leq \beta,$$

we find unitary matrices $A_n \in \mathbb{R}^{2^n \times 2^n}$ with $W(A_n) \subset W(A_{n+1}) \subset K_\beta$, and the closure of $\bigcup_n W(A_n)$ coinciding with K_β. Hence in general the relation $W(A) \subset \|A\|\, K_\beta$ cannot be improved without further knowledge on A.

We have the following result for our constrained Chebyshev approximation problem.

LEMMA 2.2. *There holds for any $k \geq 1$ for any $\beta \in (0, \pi/2)$*

$$\gamma_\beta^k < E_k(K_\beta) \leq \min\left\{2 + \gamma_\beta, \frac{2}{1 - \gamma_\beta^{k+1}}\right\} \gamma_\beta^k,$$

with $\gamma_\beta = 2\sin(\frac{\beta}{4 - 2\beta/\pi})$ as in Theorem 2.1.

Proof. Let K be some convex compact set containing at least two elements, $0 \notin K$, and denote by ϕ the Riemann conformal map mapping from $\overline{\mathbb{C}} \setminus K$ onto the exterior of the closed unit disk, with $\phi(\infty) = \infty$. In the first part of the proof we claim that

$$k \geq 1: \qquad \gamma^k \leq E_k(K) \leq \min\left\{2 + \gamma, \frac{2}{1 - \gamma^{k+1}}\right\} \gamma^k, \qquad \gamma := 1/|\phi(0)|. \tag{2.7}$$

The inequality $\gamma^k \leq E_k(K)$ follows by applying the maximum principle to the function p/ϕ^k for an arbitrary polynomial p of degree $\leq k$; see also the classical Bernstein–Walsh inequality [12]. Notice also that, again by the maximum principle, we have

$\gamma^k = E_k(K)$ for some $k > 0$ if and only if ϕ^k is a polynomial of degree k or, in other words, if K is a lemniscate, which is certainly not true for our set K_β.

For the other inequality of (2.7) we need a good candidate p of degree k. Consider the Faber polynomial F_k being the polynomial part of the Laurent expansion of ϕ^k at ∞; see, e.g., [15, 16]. It is shown in [11, Theorem 2] for general convex sets K that

$$\delta_k := \|F_k - \phi^k\|_{\partial K} \leq 1. \tag{2.8}$$

From the maximum principle applied to $\phi F_k - \phi^{k+1}$ we know that $|\phi(0)|\,|F_k(0) - \phi(0)^k| < \|\phi F_k - \phi^{k+1}\|_{\partial K} \leq \delta_k$, and hence for the polynomial depending on some parameter $v \in [0, 1]$,

$$p_v(z) = F_k(z) + v\,(\phi(0)^k - F_k(0)),$$

we obtain $|p_v(0)| \geq |\phi(0)|^k - (1-v)\delta_k/|\phi(0)|$ and

$$\|p_v\|_K = \|p_v\|_{\partial K} \leq \|\phi^k\|_{\partial K} + \|\phi^k - F_k\|_{\partial K} + v|\phi(0)^k - F_k(0)| \leq 1 + \delta_k + v\delta_k/|\phi(0)|,$$

and thus

$$E_k(K_\beta) \leq \min_{v\in[0,1]} \frac{\|p_v\|_K}{|p_v(0)|} \leq \min_{v\in[0,1]} \gamma^k \frac{1 + \delta_k(1 + v\gamma)}{1 - (1-v)\delta_k\gamma^{k+1}},$$

leading to the other inequality of (2.7).

Now the assertion of the lemma follows from (2.7) once we have shown that the Riemann conformal map ϕ for $K = K_\beta$ satisfies $1/|\phi(0)| = \gamma_\beta$. Indeed, this map can be explicitly constructed as a composition $\phi = T_3 \circ T_2 \circ T_1$, with

$$T_1(z) = \frac{z - e^{i\beta}}{z - e^{-i\beta}}, \qquad T_2(z) = (e^{i(\pi-\beta)}z)^{\pi/(2\pi-\beta)}, \qquad T_3(z) = \frac{z - \overline{T_2(1)}}{z - T_2(1)},$$

where T_1 maps the complement of K_β conformally onto $\{z \in \mathbb{C} : -\pi + \beta < \arg(z) < \pi\}$, T_2 maps $\{z \in \mathbb{C} : -\pi + \beta < \arg(z) < \pi\}$ conformally onto the upper half-plane $\{z \in \mathbb{C} : 0 < \arg(z) < \pi\}$, and finally T_3 maps the upper half-plane conformally onto the complement of the exterior of the closed unit disk. Finally, notice that

$$\frac{1}{|\phi(0)|} = \left| \frac{\exp\left(i\pi\frac{\pi+\beta}{2\pi-\beta}\right) - \exp\left(i\pi\frac{\pi-\beta}{2\pi-\beta}\right)}{\exp\left(i\pi\frac{\pi+\beta}{2\pi-\beta}\right) - \exp\left(-i\pi\frac{\pi-\beta}{2\pi-\beta}\right)} \right| = \frac{\sin\left(\frac{2\beta}{4-2\beta/\pi}\right)}{\sin\left(\frac{\pi}{2} + \frac{\beta}{4-2\beta/\pi}\right)} = \gamma_\beta,$$

as required for the assertion of Lemma 2.2. ∎

By means of elementary computations one checks that the asymptotic convergence factor $\sin(\beta)$ found by Elman coincides with $E_1(K_\beta)$, which by Lemma 2.2 is larger than our constant γ_β. Thus (2.1) is asympotically sharper than (1.1), (1.2); compare with Figures 1 and 2.

The second ingredient in our proof of Theorem 2.1 is the following observation.

LEMMA 2.3. *With $\beta \in (0, \pi/2)$ as in (1.2) there holds for any polynomial $p \neq 0$*

$$\|p(A)\| \leq (2 + 2/\sqrt{3})\,\|p\|_K, \quad K := \|A\|\,K_\beta.$$

Proof. Choose $\alpha \in (\beta, \pi/2)$, and consider the linear fractional transformation

$$r(z) = \frac{\|A\|\,e^{i\alpha} - z}{z - \|A\|\,e^{-i\alpha}}.$$

Then $f := p \circ r^{-1}$ is a rational function with all poles at $-1 \notin S_\alpha$. Also, observe that $r(K) \subset r(\|A\|\, K_\alpha) = S_\alpha$. According to the Crouzeix results (2.3) and (2.5), for the claim of Lemma 2.3 it is sufficient to show the relation $W(r(A)) \subset S_\alpha$. For a vector $y \neq 0$, we define $\tilde{y} := (A - \|A\|\, e^{-i\alpha} I)^{-1} y \neq 0$, and consider

$$\begin{aligned} d &:= \frac{(r(A)y, y)}{(\tilde{y}, \tilde{y})} = \frac{((A - \|A\|\, e^{-i\alpha} I)^*(\|A\|\, e^{i\alpha} I - A)\tilde{y}, \tilde{y})}{(\tilde{y}, \tilde{y})} \\ &= -\|A\|^2\, e^{2i\alpha} - \frac{\|A\tilde{y}\|^2}{\|\tilde{y}\|^2} + 2\,\|A\|\, e^{i\alpha}\, \mathrm{Re}\left(\frac{(A\tilde{y}, \tilde{y})}{(\tilde{y}, \tilde{y})}\right). \end{aligned}$$

Thus $\mathrm{Im}(d) \geq 2\,\|A\|^2 \sin(\alpha)[-\cos(\alpha) + \cos(\beta)] > 0$, and $\mathrm{Im}(e^{-i\alpha} d) = \sin(\alpha)\, [-\|A\|^2 + \|A\tilde{y}\|^2/\|\tilde{y}\|^2] \leq 0$, implying that $W(r(A)) \subset S_\alpha$. ◻

Since the quantity $E_k(K)$ is invariant under a scaling of the set K, we obtain from Lemma 2.3

$$\begin{aligned} &\min\{\|p(A)\| : p \text{ a polynomial of degree} \leq k,\, p(0) = 1\} \\ &\leq (2 + 2/\sqrt{3})\, E_k(\|A\|\, K_\beta) = (2 + 2/\sqrt{3})\, E_k(K_\beta), \end{aligned}$$

and Lemma 2.2 allows us to conclude the proof of Theorem 2.1.

Since the method of proof of (2.7) does not depend on the particular choice of the shape of the domain including the field of values, we have shown implicitly the following result complementary to Theorem 2.1 (compare with [3, section 9]).

COROLLARY 2.4. *Let K be some compact convex set not including the origin, and let A be some matrix with $W(A) \subset \|A\|\, K$. Then for the kth relative residual, $k \geq 1$, of GMRES we have*

$$\frac{\|r_k\|}{\|r_0\|} \leq [2 + \gamma]\, C(K)\, \gamma^k < [2 + \gamma]\, C(K)\, E_k(K),$$

where $C(K)$ can be chosen as in (2.4) or in (2.6), and $\gamma = 1/|\phi(0)| < 1$, ϕ denoting the Riemann conformal map mapping from $\overline{\mathbb{C}} \setminus K$ onto the exterior of the unit disk, with $\phi(\infty) = \infty$.

In particular, we get from Corollary 2.4 that the norm of the kth relative residual of GMRES is bounded above by $101.25\,\gamma^k$, with $\gamma < 1$ as before.

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Note added in proof. After finishing this paper, one of the authors [2] was able to show an improvement of Corollary 2.4: For a convex compact set E and a matrix A with $W(A) \subset E$ it is shown in [2, Theorem 1] that $\|F_n(A)\| \leq 2$, where F_n denotes the nth Faber polynomial corresponding to the set E. As a consequence [2, Theorem 2 and Corollary 3], Corollary 2.4 remains valid after replacing the constant $C(K)$ by 1.

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