Some remarks on the Elman estimate for GMRES

by

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Abstract

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

Key words: GMRES, non-symmetric systems, error estimates, field of values.
AMS Classification (2000): 65F10, 65N22

1 Introduction

A popular method for solving non-hermitian systems $Ax = b$ is given by GMRES [10]. Provided that A has a positive definite hermitian part $(A + A^*)/2$, Elman [6] pointed out the following upper bound for the norm of the kth residual r_k of GMRES for every $k \geq 0$

$$\frac{||r_k||}{||r_0||} \leq \sin^k(\beta), \qquad \text{where } \beta \in [0, \pi/2] \text{ is defined by } \cos(\beta) := \frac{\lambda_{\min}((A + A^*)/2)}{||A||}. \qquad (1)$$

Here and hereafter we use $||\cdot||$ to denote 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 $\mathrm{dist}(0, W(A)) = \lambda_{\min}((e^{it}A + (e^{it}A)^*)/2)$, and $t = 0$ 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) as

$$k \geq 0 : \qquad \frac{||r_k||}{||r_0||} \leq \sin^k(\beta), \qquad \cos(\beta) \leq \frac{\mathrm{dist}(0, W(A))}{||A||}, \qquad (2)$$

where we recall that (2) can be sharper than (1).

Estimates (1) or (2) are obtained by iterating the inequality for $k = 1$ corresponding to a one-dimensional minimization problem, which should allow for some improvements. 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.
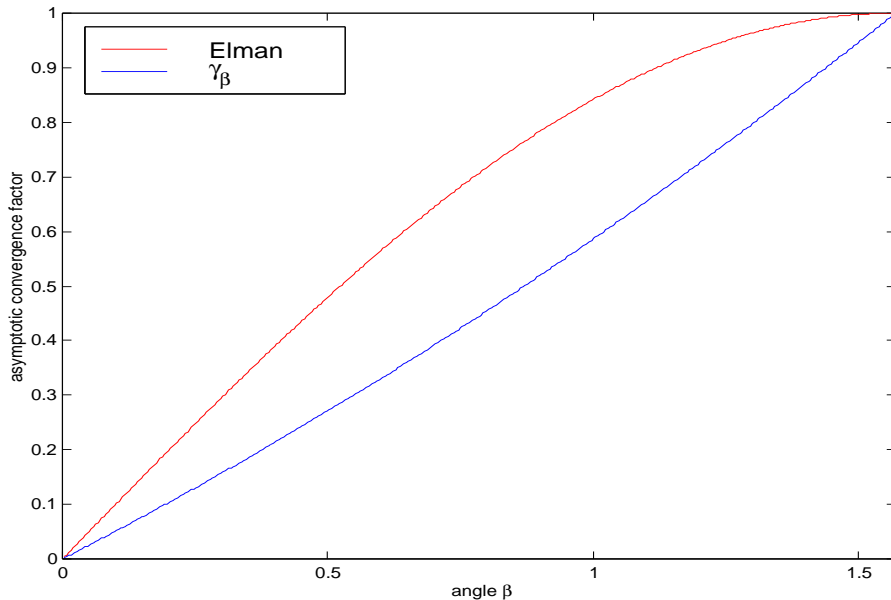
Figure 1: *Elman's asymptotic convergence factor* $\sin(\beta)$ *versus the new asymptotic convergence factor* γ_β *of Theorem 1.*

2   Main result

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

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

where

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

All convergence bounds (1), (2), (3) 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) and of Theorem 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 1 is clearly more interesting. However, the constant factor of (3) (which can be shown to be not optimum) slightly deteriorates the sharpness of the new convergence bound, see Figure 2.

Before entering in the proof of Theorem 1, let us briefly recall some well-known facts on the convergence of GMRES. Starting from the observation

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

there are many classical GMRES estimates not involving special properties of the right-hand side b of the system, see for instance [11, Chapter 6.11] or [7, Chapter 3]. Here usually the quantity on the right is estimated in terms of a polynomial extremal problem: for a compact set K, consider the constrained Chebyshev approximation problem

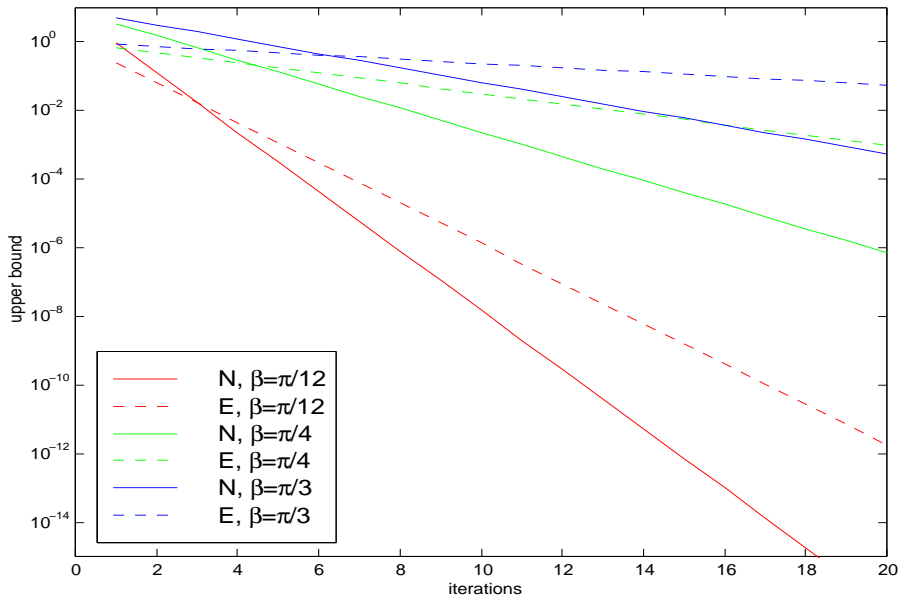$$E_k(K) := \min\{||p||_K : p \text{ a polynomial of degree} \leq k,\ p(0) = 1\},$$

Figure 2: *Upper bounds for the relative residuals of the kth iterate ($k = 1, ..., 20$) of GMRES for three different values of β (E=Elman's bound, N=bound of Theorem 1).*

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

$$k \geq 0: \qquad \frac{||r_k||}{||r_0||} \leq ||V|| \, ||V^{-1}|| \, E_k(\sigma(A)) \tag{4}$$

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 pseudo-spectrum, but in general the shape of these sets are difficult to predict. A third group of estimates are obtained via the field of values, starting perhaps with a paper of Eiermann [5], see also [7]. 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

$$W(A) \subset K \qquad \Longrightarrow \qquad ||f(A)|| \leq C(K) \, ||f||_K. \tag{5}$$

Recently, Crouzeix and his co-workers [1, 2, 3, 4] gave quite deep results concerning (5). For instance, the existence of a such finite constant in (5) only depending on the set K was established in [4]. In [1, Corollary 2.3], it was shown that for the optimal constant in (5) (also denoted by $C(K)$) one has

$$C(K) \leq 2 + \pi + \int_0^{2\pi} \frac{|\rho'(t)|}{\rho(t)} \, dt, \tag{6}$$

where $[0, 2\pi] \ni t \mapsto z_0 + \rho(t)e^{it} \in \partial K$ with $\rho(t) > 0$ 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 A is hermitian and thus $C(K) = 1$). The authors also give improved estimates for particular K, e.g., for a sector [3]

$$C(S_\alpha) \leq 2 + 2/\sqrt{3}, \qquad S_\alpha = \{z \in \mathbb{C} : 0 \leq \arg(z) \leq \alpha\}, \quad 0 \leq \alpha \leq \pi. \tag{7}$$

In some recent manuscript [2], Crouzeix showed that

$$C(K) \leq 33.75 \tag{8}$$

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for any convex compact set K, independently of its shape. It is a conjecture of Crouzeix that $C(K)$ in (5) can be replaced by the number 2.

Let us return to the proof of Theorem 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

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

with β as in (2). Define K_β to be the (convex) intersection between the closed unit disk and the half plane $\{\text{Re}(z) \geq \cos(\beta)\}$. 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. *There holds for any $k \geq 1$ for any $\beta \in (0, \pi/2)$*

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

with $\gamma_\beta = 2\sin(\frac{\beta}{4 - 2\beta/\pi})$ as in Theorem 1.

Proof. Let K be some convex compact set different from a disk containing at least 2 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

$$k \geq 1: \qquad \gamma^k \leq E_k(K) \leq \min\{2 + \gamma, \frac{2}{1 - \gamma^{k+1}}\} \gamma^k, \qquad \gamma := 1/|\phi(0)|, \tag{9}$$

and $\gamma^k < E_k(K)$ unless K is a lemniscate. 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 [9]. Moreover, 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 if and only if K is a lemniscate, which was excluded,

For the other inequality of (9) we need a good candidate p of degree k. Consider the Faber polynomial F_k being the polynomial part of ϕ^k, see, e.g., [12, 13]. It is shown in [8, Theorem 2] for general convex sets K that
$$\delta_k := ||F_k - \phi^k||_{\partial K} \leq 1. \tag{10}$$
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

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

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

leading to the other inequality of (9). Now the assertion of the Lemma follows from (9) by observing that the Riemann conformal map for $K = K_\beta$ can be explicitly constructed [12], given by $\phi = T_3 \circ T_2 \circ T_1$, with

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

and in particular

$$1/|\phi(0)| = \gamma_\beta.$$

$\square$

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 is larger than our constant γ_β. Thus (3) is asympotically sharper than (1), (2), compare with Figure 1 and Figure 2.

The second ingredient in our proof of Theorem 1 is the following observation.

Lemma 3. *With $\beta \in (0, \pi/2)$ as in (2) there holds for any polynomial $p \ne 0$*

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

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 (5) and (7), for the claim of Lemma 3 it is sufficient to show the relation $W(r(A)) \subset S_\alpha$. For a vector $y \ne 0$, we define $\tilde{y} := (A - ||A||\,e^{-i\alpha}I)^{-1}y \ne 0$, and consider

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

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

Since the quantity $E_k(K)$ is invariant under a scaling of the set K, we obtain from Lemma 3

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

and Lemma 2 allows to conclude the proof of Theorem 1.

Since the method of proof of (9) 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 1 (compare with [2, Section 9]).

Corollary 4. *Let K be some compact convex set not including the origin, and A 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 (6) or in (8), 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 4 that the kth relative residual of GMRES is bounded above by $101.25 \, \gamma^k$, with $\gamma < 1$ as before.

Acknowledgements

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