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GMRES VS. IDEAL GMRES*

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Abstract. The GMRES algorithm minimizes $\|p(A)b\|$ over polynomials p of degree n normalized at $z = 0$. The ideal GMRES problem is obtained if one considers minimization of $\|p(A)\|$ instead. The ideal problem forms an upper bound for the worst-case true problem, where the GMRES norm $\|p_b(A)b\|$ is maximized over b. In work not yet published, Faber, Joubert, Knill, and Manteuffel have shown that this upper bound need not be attained, constructing a 4×4 example in which the ratio of the true to ideal GMRES norms is 0.9999. Here, we present a simpler 4×4 example in which the ratio approaches zero when a certain parameter tends to zero. The same example also leads to the same conclusion for Arnoldi vs. ideal Arnoldi norms.

Key words. GMRES, ideal GMRES, Arnoldi, ideal Arnoldi

AMS subject classifications. 65F10, 49K35

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1. Introduction.

The GMRES algorithm [7] is an iterative method for solving non-hermitian linear systems $Ax = b$ ($A \in \mathbb{C}^{N\times N}$, $b \in \mathbb{C}^N$). Throughout this paper, $\mathbb{C}^N$ is given the 2-norm $\|\cdot\|$ and $\mathbb{C}^{N\times N}$ is given the corresponding induced matrix norm. Each step (say the nth) of the GMRES algorithm is mathematically equivalent[1] to minimizing $\|p(A)b\|$ over the polynomials in P_n, where

$$P_n = \{\text{polynomials of degree} \leq n \text{ with } p(0) = 1\}.$$

For each b, the GMRES polynomial (denoted by p_b) exists and is unique if $\|p_b(A)b\| > 0$.

How fast a GMRES iteration converges, i.e., how fast $\|p_b(A)b\|$ converges to zero as n increases, depends on the matrix A and the vector b. In practice, however, unless b has special properties, it appears to be usually A that predominantly determines the convergence rate. To understand how the GMRES convergence rate depends on A without the complicating effect of the right-hand side vector, Greenbaum and Trefethen [5] introduced the "ideal GMRES matrix approximation problem": minimization of $\|p(A)\|$ over polynomials in the same class P_n. The "ideal GMRES polynomial," which we will denote by p_*, exists and is unique so long as $\|p_*(A)\| > 0$. To avoid possible confusion, we will refer to GMRES as true GMRES.

The ideal GMRES convergence curve forms an upper bound for the true GMRES convergence curves in the sense that for each n,

$$\max_{b\in\mathbb{C}^N,\ \|b\|=1} \|p_b(A)b\| \leq \|p_*(A)\|. \tag{1.1}$$

This inequality is actually an equality for many matrices, including normal matrices [3], [4], triangular Toeplitz matrices with $p_*(z) = 1$ [2], and matrices A whose ideal GMRES matrix $p_*(A)$ has a simple maximal singular value [5]. It is also an equality for

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[1]We have assumed, without loss of generality, that the initial guess for the iteration is $x_0 = 0$.

arbitrary matrices at step $n = 1$ [3],[4]. Positive results such as these led Greenbaum and Trefethen [5] to conjecture that (1.1) was an equality, i.e., "the ideal GMRES bound is attained," for every matrix A. However, at the 1994 Colorado Conference on Iterative Methods at Breckenridge, Colorado, Faber, Joubert, Knill, and Manteuffel presented a counterexample to this conjecture [2]. Their example is a dense 4×4 matrix constructed using the theory of generalized fields of values, where the inequality (1.1) is strict at step $n = 3$. The degree-3 ideal GMRES polynomial for their example is $p_*(z) = 1$; hence $\|p_*(A)\| = 1$. The corresponding quantity on the left-hand side of (1.1) is 0.99988.

We have found a simpler (bidiagonal) family of 4×4 matrices that can achieve arbitrarily small ratio when a certain parameter in the family tends to zero. The purpose of this short paper is to present this example and speculate briefly on its significance.

2. The counterexample: Mathematical proof. Our counterexample is the 4×4 matrix

$$A = \begin{pmatrix} 1 & \epsilon & & \\ & -1 & c/\epsilon & \\ & & 1 & \epsilon \\ & & & -1 \end{pmatrix}, \quad \epsilon > 0, \quad 0 < c < 2. \tag{2.1}$$

We would like to note that the parameter c in the example is not crucial to establishing our goal, namely, to show that the worst-case true and ideal GMRES norms in (1.1) differ. However, it gives us the freedom to construct examples with an ideal GMRES norm anywhere between zero and one. For simplicity, the reader can assume c to be one.

THEOREM 2.1. *For the matrix A of* (2.1)*, the degree-*3 *ideal GMRES polynomial is*

$$p_*(z) = 1 + (\alpha - 1)z^2 \tag{2.2}$$

with

$$\alpha = \frac{2c^2}{4 + c^2}. \tag{2.3}$$

The corresponding matrix is

$$p_*(A) = \begin{pmatrix} \alpha & 0 & \gamma & \\ & \alpha & 0 & \gamma \\ & & \alpha & 0 \\ & & & \alpha \end{pmatrix},$$

where

$$\gamma = (\alpha - 1)c, \tag{2.4}$$

with norm

$$\|p_*(A)\| = \frac{4c}{4 + c^2}. \tag{2.5}$$

Proof. Since A is real, we have $\|p(A)\| = \|\bar{p}(A)\|$ for any p. Uniqueness of the ideal GMRES polynomial then implies that $p_*(z) = \bar{p}_*(z)$, i.e., the coefficients of $p_*(z)$ are real. Next we observe that A^T is unitarily similar to $-A$ via the matrix

$$Q = \begin{pmatrix} & & & -1 \\ & & 1 & \\ & -1 & & \\ 1 & & & \end{pmatrix};$$

i.e., $-A = QA^TQ^{-1}$. This implies that $\|p(-A)\| = \|p(A^T)\| = \|p(A)\|$ for any p. By uniqueness, again, we have $p_*(-z) = p_*(z)$; i.e., p_* is even.

Now consider polynomials of the form (2.2), viewing α as a real parameter. For a given pair of ϵ and c, we can find the singular values of $p(A)$ analytically as a function of α:

$$\sigma^2_{\max}(\alpha) = \frac{1}{2}\left(2\alpha^2 + \gamma^2 + |\gamma|\sqrt{4\alpha^2+\gamma^2}\right), \tag{2.6}$$

$$\sigma^2_{\min}(\alpha) = \frac{1}{2}\left(2\alpha^2 + \gamma^2 - |\gamma|\sqrt{4\alpha^2+\gamma^2}\right), \tag{2.7}$$

with γ related to α and c by (2.4). Each of these singular values has multiplicity two. The value of α corresponding to the ideal GMRES polynomial $p_*(z)$ is the value for which $\sigma^2_{\max}(\alpha)$ is minimum. Now we have a calculus problem; we can simply differentiate (2.6) with respect to α and set the derivative to zero. This gives us the formula (2.3) for α as a function of c; we omit the details. The corresponding singular values of $p_*(A)$ are

$$\sigma_{\max} = \frac{4c}{4+c^2}, \qquad \sigma_{\min} = \frac{c^3}{4+c^2}. \tag{2.8}$$

A biorthogonal set of basis vectors for the maximal left and right singular spaces of $p_*(A)$ is

$$U_1 = \begin{pmatrix} 0 & 2 \\ 2 & 0 \\ 0 & -c \\ -c & 0 \end{pmatrix}, \qquad V_1 = \begin{pmatrix} 0 & c \\ c & 0 \\ 0 & -2 \\ -2 & 0 \end{pmatrix}. \tag{2.9}$$

In what follows, we will denote the columns of U_1 and V_1, respectively, by u_i $(i = 1, 2)$ and v_i $(i = 1, 2)$. $\square$

Remark. The results of Theorem 2.1 are valid only for $0 < c < 2$. However we may extend these results to the case $c = 2$, since $p_*(A)$ is a continuous function of c. For example, by letting c tend to two in (2.2), we have $p_*(z) = 1$ and hence $\|p_*(A)\| = 1$.

It is easily shown that for our matrix A, the worst-case true and ideal GMRES norms differ. Before attempting to quantify this difference, we will show that it exists.

THEOREM 2.2. *Suppose A is given by* (2.1). *Then for any vector $b \in \mathbb{C}^4$, the corresponding degree-*3 *true GMRES polynomial p_b for A satisfies $\|p_b(A)b\| < \|p_*(A)\|\|b\|$.*

Proof. We prove this by contradiction. Suppose the envelope is attained, i.e., equality holds in (1.1) for some b. It is easily shown that b must be a maximal right singular vector of $p_*(A)$. That is, it lies in the span of v_1 and v_2, and the corresponding true GMRES polynomial must be $p_*(z)$ itself. Without loss of generality, we can assume that b has the form $b = \beta_1 v_1 + \beta_2 v_2$, where β_1, β_2 are not both zero. Since p_b is a true GMRES polynomial for b, it is readily shown that $p_*(A)b$ must satisfy the orthogonality conditions

$$\langle A^k b,\, p_*(A)b\rangle = 0, \quad k = 1, 2, 3.$$

Noting that $p_*(A)v_i = \sigma_{\max} u_i,\ i = 1, 2$ and evaluating the inner products for $k = 1$ and 3 gives

$$-4c\,|\beta_1|^2 + 4c\,|\beta_2|^2 - 4\frac{c}{\epsilon}\,\bar\beta_1\beta_2 + 4c\epsilon\,\beta_1\bar\beta_2 = 0, \tag{2.10}$$

$$-4\frac{c}{\epsilon}\,\bar\beta_1\beta_2 = 0. \tag{2.11}$$

Equation (2.11) implies that $\beta_1 = 0$ or $\beta_2 = 0$. In either case, substitution into (2.10) gives $c = 0$. Since $c \neq 0$, we have a contradiction. ∎

Our larger goal is to show that the worst-case true and ideal GMRES norms do not merely differ but can have a ratio arbitrarily small. For this we can use the following more quantitative argument.

THEOREM 2.3. *Suppose A is given by* (2.1) *with* $0 < \epsilon \le 1$. *Then*

$$\max_{\|b\|=1} \|p_b(A)b\| \le 2(1+c)\sqrt{\epsilon} \;+\; (2+3c)\epsilon. \tag{2.12}$$

Thus for each $0 < c < 2$*,*

$$\frac{\max_{\|b\|=1}\ \|p_b(A)b\|}{\|p_*(A)\|} \longrightarrow 0 \quad \text{as} \ \ \epsilon \to 0. \tag{2.13}$$

Proof. We will show that for each $b \in \mathbb{C}^4$ with $\|b\| = 1$, there exists a polynomial $p \in P_n$ such that $\|p(A)b\|$ is less than or equal to the right-hand side of (2.12). Then (2.12) follows from the optimality property of GMRES.

Let $b = (b_1, b_2, b_3, b_4)^T$. We have

$$Ab = \begin{pmatrix} b_1 \\ -b_2 + cb_3/\epsilon \\ b_3 \\ -b_4 \end{pmatrix} + \epsilon \begin{pmatrix} b_2 \\ 0 \\ b_4 \\ 0 \end{pmatrix}, \quad A^2 b = b + c \begin{pmatrix} b_3 \\ b_4 \\ 0 \\ 0 \end{pmatrix},$$

$$A^3 b = Ab + c \begin{pmatrix} b_3 \\ -b_4 \\ 0 \\ 0 \end{pmatrix} + c\epsilon \begin{pmatrix} b_4 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Consider polynomials $p \in P_n$ of the form

$$p(z) = 1 + \xi z - z^2 + (\eta - \xi) z^3.$$

Then

$$p(A)b = \begin{pmatrix} -cb_3 \;+\; (\eta-\xi)cb_3 \;+\; \eta b_1 \\ -cb_4 \;-\; (\eta-\xi)cb_4 \;-\; \eta b_2 \;+\; \eta c b_3/\epsilon \\ \eta b_3 \\ -\eta b_4 \end{pmatrix} \;+\; \epsilon\, r,$$

where

$$r = \eta \begin{pmatrix} b_2 \\ 0 \\ b_4 \\ 0 \end{pmatrix} + (\eta - \xi) c \begin{pmatrix} b_4 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Now we have two cases to consider. For each, we will show that $\|p(A)b\|$ is less than or equal to the right-hand side of (2.12) with appropriately chosen ξ and η.

Case 1. Suppose $|b_3| \geq \sqrt{\epsilon}$. Take $\xi = -1$ and $\eta = 2\epsilon b_4/b_3$. Then $|\eta| \leq 2\sqrt{\epsilon}$ and

$$p(A)b = \eta \begin{pmatrix} b_1 + cb_3 \\ -b_2 - cb_4 \\ b_3 \\ -b_4 \end{pmatrix} + \epsilon\, r.$$

Hence

$$\|p(A)b\| \;\leq\; (1+c)\,|\eta| \,+\, (2+3c)\,\epsilon \;\leq\; 2(1+c)\sqrt{\epsilon} \,+\, (2+3c)\,\epsilon.$$

Case 2. Suppose $|b_3| \leq \sqrt{\epsilon}$. Take $\xi = 1$ and $\eta = \epsilon$. Then

$$p(A)b = c \begin{pmatrix} -2b_3 \\ b_3 \\ 0 \\ 0 \end{pmatrix} + \eta \begin{pmatrix} b_1 + cb_1 \\ -b_2 - cb_4 \\ b_3 \\ -b_4 \end{pmatrix} + \epsilon\, r.$$

Thus

$$\begin{aligned} \|p(A)b\| &\leq \sqrt{5}c\,|b_3| \,+\, (1+c)\,|\eta| + (1+2c)\,\epsilon \\ &\leq 2(1+c)\sqrt{\epsilon} \,+\, (2+3c)\,\epsilon. \qquad \square \end{aligned}$$

Remark. Note that (2.12) in fact holds for all $c > 0$. Since $\|p_*(A)\| = 1$ for all $\epsilon > 0$ when $c = 2$, as a result (2.13) also holds for $c = 2$.

3. The counterexample: Numerical evidence. Theorem 2.3 shows that the ratio of the true to ideal GMRES norms for our matrix A is no greater than order $\sqrt{\epsilon}$ as $\epsilon \to 0$. In fact, numerical experiments indicate that this square root dependence is sharp. We have used the MATLAB optimization routine `fminu` [6] to maximize $\|p_b(A)b\|$ over $b \in \mathbb{C}^4$ with $\|b\| = 1$. To ensure that we have the global maximum for the worst-case true GMRES, numerous trails with different initial guesses are carried out with `fminu`. The ideal GMRES polynomial is computed from (2.2).

Figure 3.1 plots the ratio between the worst-case true GMRES and the ideal GMRES norms for the matrix A of (2.1) with $0 < \epsilon \leq 10$ and $c = 1$. The dashed curve shows an upper bound on the ratio obtained by dividing the right-hand quantity of (2.12) by the ideal GMRES norm of A in (2.5). The slope of the curves in the figure is 0.5.

By extending the matrix A of (2.1) to higher dimensions, say to an even integer N (with ± 1 alternating along the diagonal and ϵ, c/ϵ alternating along the first superdiagonal), we obtain examples where the ideal GMRES envelope is not attained at step $n = N - 1$. For such matrices, again, the ideal GMRES polynomials do not depend on ϵ. We have used codes provided by Michael Overton to compute the ideal GMRES polynomials. Numerical experiments also indicate that the worst-case true GMRES norms at step $n = N - 1$ are no greater than order $\sqrt{\epsilon}$ as $\epsilon \to 0$. Thus the ratio between the worst-case true GMRES and ideal GMRES norms at step $n = N-1$ approaches zero as ϵ tends to zero.

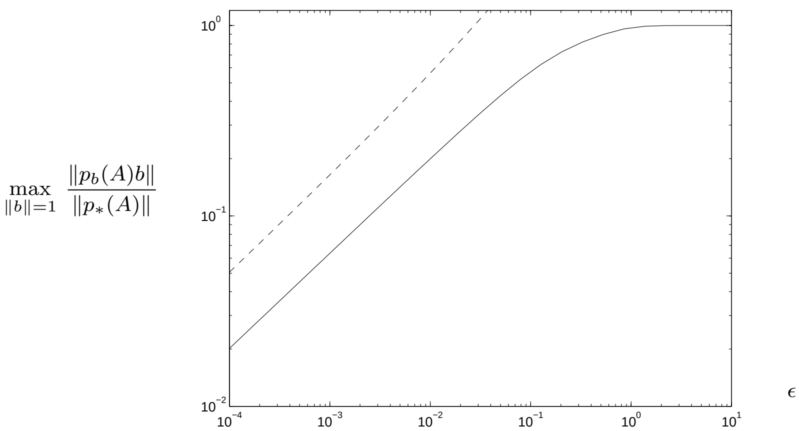

Fig. 3.1. *Ratio between the worst-case true GMRES and ideal GMRES norms at step* $n = 3$ *for the matrix* A *of* (2) *with* $c = 1$*, as a function of* ϵ *(numerically computed). The plateau portion of the solid curve is strictly below* 1 *for all* ϵ*, by Theorem* 2.2*. The dashed curve represents the upper bound of Theorem* 2.3.

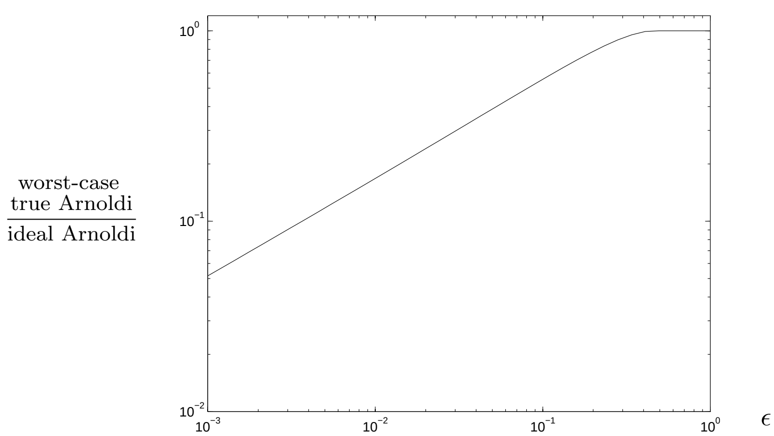

Fig. 4.1. *Analogous plot for true vs. ideal Arnoldi approximation of the same matrix* A *with* $c = 1$*. The ratio is exactly* 1 *for* ϵ *approximately greater than* 0.459.

4. Discussion. The true and ideal Arnoldi problems are the analogs of the true and ideal GMRES problems, except that the minimizations are over the class of monic polynomials of degree $\leq n$ instead of P_n. Numerical evidence again suggests that for the matrix A of (2.1), the ratio between the worst-case true Arnoldi and the ideal Arnoldi norms at step $n = 3$ approaches zero as ϵ tends to zero. Figure 4.1 plots the ratio associated with the Arnoldi problems for our matrix A with $10^{-3} \leq \epsilon \leq 1$ and $c = 1$.

Finally, we must raise the question of the practical significance of our results. Greenbaum and Trefethen [5], as well as others, have assumed that for most nonsymmetric matrix iterations in most applications, convergence rates can be analyzed in terms of a matrix approximation problem. Our result introduces the possibility that this might not be true. There may be applications in which Krylov subspace iterations perform much better than analysis of matrix approximation problems can explain, and conceivably, such applications might be common. Our guess is that this will not prove to be the case, but it must be admitted that at the moment there is very little evidence one way or the other.

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