The worst-case GMRES for normal matrices

J. Liesen and P. Tichý

Technical University of Berlin, Berlin
Academy of Sciences of the Czech Republic, Prague

1 Introduction

Convergence analysis of GMRES has been an active area of research since the algorithm's introduction, and numerous papers have been devoted to this subject. When the system matrix is normal, the earliest upper bound on the GMRES residual norms (henceforth called the "standard bound") represents a certain min-max approximation problem on the set of the matrix eigenvalues. Being independent of the initial residual, the standard bound is in fact a bound on the "worst-case" GMRES residual norms for the given system matrix. For normal matrices the standard bound has been shown to be sharp in the sense that for each GMRES iteration step there exists an initial residual (depending on the matrix and the iteration step) for which the bound is attained [2]. In the talk we explore this standard bound.

2 Basic concepts

Let a linear system

$$Ax = b\,, \tag{1}$$

with a *nonsingular and normal* matrix $A \in \mathbb{C}^{n\times n}$ and $b \in \mathbb{C}^n$ be given. Furthermore, let $A = Q\Lambda Q^H$ be the eigendecomposition of A, where $Q^H Q = I$, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, and let $L = \{\lambda_1, \ldots, \lambda_n\}$ denote the set of all eigenvalues of A. To avoid unnecessary technical complications we will assume that *all eigenvalues of A are distinct*.

Suppose that we solve (1) with GMRES. Starting from an initial guess x_0, this method computes the initial residual $r_0 = b - Ax_0$ and a sequence of iterates $x_1, x_2, \ldots$, so that the ith residual $r_i \equiv b - Ax_i$ satisfies

$$\|r_i\| \;=\; \min_{p\in\pi_i} \|p(A)\, r_0\|\,, \tag{2}$$

where π_i denotes the set of polynomials of degree at most i and with value one at the origin, and $\|\cdot\|$ denotes the 2-norm. Assuming that $\|r_0\| = 1$, the standard upper bound on the GMRES residual norms follows easily from (2),

$$\|r_i\| \;\le\; \min_{p\in\pi_i} \max_{\lambda_j\in L} |p(\lambda_j)|. \tag{3}$$

As shown in [2], for each normal matrix A and each step i, there exists an initial residual $r_0^{(i)}$ so that equality holds in (3). We introduce the following definition.

Definition: An ith worst-case GMRES residual r_i^w for $A \in \mathbb{C}^{n\times n}$ is a GMRES residual that satisfies

$$\|r_i^w\| \;=\; \max_{\|r_0\|=1} \min_{p\in\pi_i} \|p(A)\, r_0\|\,, \qquad i = 1, \ldots, n-1.$$

The sharpness of the bound (3) sometimes leads to the impression that the GMRES convergence behavior for normal matrices is fully understood. However, the solution of the min-max approximation is in general unknown and its known estimates based on only a few properties of the matrix (such as the condition number) are often misleading. Here we consider this problem and characterize the standard bound in terms of easily comprehensible expressions involving the matrix eigenvalues.

3 GMRES residual in the next-to-last step

We parameterize the initial residual r_0 by

$$r_0 \;=\; Q\,[\varrho_1, \ldots, \varrho_n]^T\,.$$

Considering that $\varrho_j \neq 0$ for all j, we proved in [1] that the norm of the $(n-1)$st GMRES residual r_{n-1} satisfies

$$\|r_{n-1}\| \;=\; \left(\sum_{j=1}^{n} \left|\frac{l_j(0)}{\varrho_j}\right|^2\right)^{-1/2}, \tag{4}$$

where $l_j(\lambda)$ is the jth Lagrange polynomial,

$$l_j(\lambda) \;\equiv\; \prod_{\substack{k=1\\k\neq j}}^{n} \frac{\lambda_k - \lambda}{\lambda_k - \lambda_j}\,.$$

Speaking about the worst-case GMRES residual norm in the $(n-1)$st iteration step, we have to maximize the $(n-1)$st residual norm (4). This can be done by using Cauchy's inequality. In [1] we showed that the norm of the $(n-1)$st worst-case GMRES residual r_{n-1}^w is given by

$$\|r_{n-1}^w\| \;=\; \left(\sum_{k=1}^{n} |l_k(0)|\right)^{-1}. \tag{5}$$

4 Worst-case GMRES residual in a general step i

For each subset S of the eigenvalues of A, $S \subseteq L$ with $i+1$ elements we denote

$$M_i^S \;\equiv\; \min_{p\in\pi_i} \max_{\lambda_j\in S} |p(\lambda_j)| \;=\; \left(\sum_{k=1}^{i+1} |l_k^S(0)|\right)^{-1},$$

where $l_k^S(\lambda)$, denotes the kth Lagrange polynomial corresponding to the elements in the set S. For $S = L$ and $i = n-1$, this value is the worst-case residual norm in the next-to-last step, cf. (5). In a general step i,

$$\|r_i^w\| \;=\; M_i^L \;\geq\; M_i^S \quad\Rightarrow\quad M_i^L \;\geq\; \max_{\substack{S\subseteq L\\|S|=i+1}} M_i^S \;\equiv\; B_i^L,$$

where B_i^L represents a computable lower bound. We can ask how close is B_i^L to M_i^L.

When all eigenvalues forming the set L are real, then it follows from a classical result of approximation theory that

$$B_i^L \;=\; \|r_i^w\|\,.$$

When L contains at least one non-real eigenvalue, we don't have equality in general and B_i^L is only a lower bound. In our paper [1] we proved an upper bound. We showed that the worst-case residual norm can be bounded by

$$B_i^L \;\leq\; \|r_i^w\| \;\leq\; \sqrt{(i+1)(n-i)}\; B_i^L\,. \tag{6}$$

Our numerical experiments with various spectra show that the lower bound B_i^L is very tight and that the upper bound (6) represents an overestimation. In particular, we *conjecture* that there exists a small constant $C > 1$ such that

$$B_i^L \;\leq\; \|r_i^w\| \;\leq\; C\, B_i^L$$

holds for *all* sets L containing n distinct complex numbers.

5 Numerical experiments

To justify our conjecture, we present some numerical experiments. In the first numerical experiment we consider the eigenvalue set L consisting of the 18th roots of unity. In this case worst-case GMRES completely stagnates, which is confirmed by the bold line in Figure 1. The lower bound B_i^L closely approximates the worst-case residual norm, and the lower bound multiplied by $4/\pi$ represents an upper bound. As shown in [1], the lower bound approaches $\pi/4$ from above in the step $i = n - 2$ (here: $i = 16$) when $n \to \infty$. Hence in this step the lower bound multiplied by $4/\pi$ is proven to be a (sharp) upper bound on the worst-case GMRES. The tightness of this bound, even for the moderate $n = 18$, is clearly visible in Figure 1.

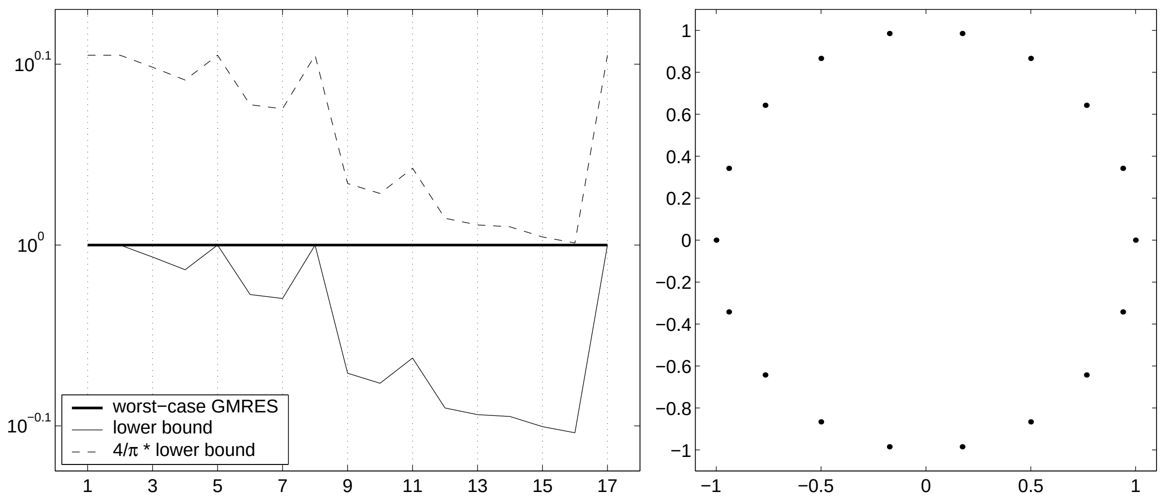

Figure 1: Worst-case GMRES and our bounds for roots of unity.

In the case of random eigenvalues in the region $[0, 1] \times \mathbf{i}\,[0, 1]$, the convergence of the worst-case residual norms is moderately fast; they decrease about 4 orders of magnitude until the next-to-last step, cf. Figure 2. Again the lower bound B_i^L is a good estimate (bold and solid line almost coincide), and the dashed line represents an upper bound.

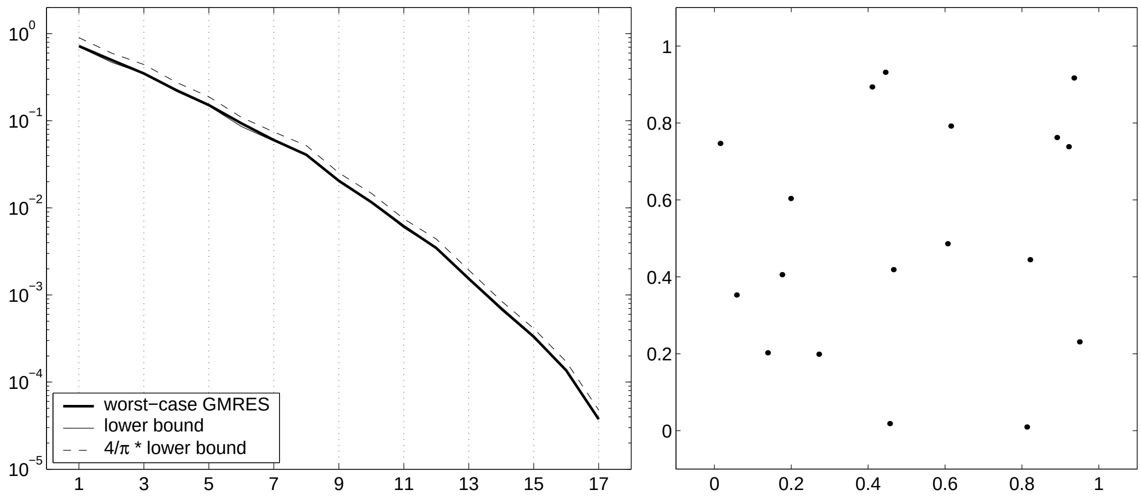

Figure 2: Worst-case GMRES and our bounds for random eigenvalues in the region $[0, 1] \times \mathbf{i}\,[0, 1]$.

6 Conclusions

We completely characterized the GMRES residual norm and also the worst-case GMRES residual norm in the $(n-1)$st iteration step. For a general step i, the worst-case GMRES residual norm can be estimated by a computable value B_i^L. In particular, the worst-case GMRES residual norm is equal to B_i^L when A has real eigenvalues and B_i^L is a lower bound in the case of complex eigenvalues. Numerical experiments predict that this lower bound is very tight and is up to factor of $4/\pi$ equal to B_i^L. Naturally, the determination of the value B_i^L represents a theoretical problem but it can help us to analyze the convergence of GMRES for model problems where the eigenvalues are known.

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References

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