Computable convergence bounds for GMRES

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Abstract

The main purpose of this paper is the derivation of computable bounds on the residual norms of (full) GMRES. The new bounds depend on the initial guess and thus are conceptually different from standard 'worst-case' bounds. The analysis is valid for nonsingular linear systems and for any singular linear system, provided a certain condition on the initial residual is satisfied. It is shown that approximations to all factors in the new bounds can be obtained early in the GMRES run. The approximations serve to predict the convergence behavior of GMRES in later phases of the iteration. Numerical examples demonstrate that the new bounds are capable to describe the actual convergence behavior of GMRES for the given linear system and initial guess.

Key words. linear systems, convergence analysis, GMRES method, Krylov subspace methods, iterative methods

AMS Subject Classifications. 65F10, 65F15, 65F50, 65N12, 65N15

1 Introduction

The GMRES algorithm by Saad and Schultz [22] is one of the most popular iterative methods for solving a system of linear equations,

$$A\hat{x} = b,\ A \in \mathbf{C}^{N\times N},\ b \in \mathbf{C}^{N}. \tag{1.1}$$

The convergence analysis of GMRES has been an attractive field of research in recent years. Among others, Saad and Schultz [22], Nachtigal, Reddy and Trefethen [19], Starke [24] and Eiermann [7] derived upper bounds on the residual norms. However, none of these bounds leads to a complete characterization of the algorithm's convergence behavior. Some bounds are only applicable to a restricted class of nonsingular linear systems, others include factors that are not computable. All of these bounds are independent of the initial guess. As demonstrated in examples by Faber et al. [10] and Toh [27] this might lead to an over-estimation even of the algorithm's worst-case behavior. It is generally agreed, that the convergence analysis of GMRES needs further work (see e.g. [25, p. 187]).

In response, this paper tries to shed more light on the situation. Based on new characterizations of GMRES-equivalent matrices, we derive new convergence results for GMRES, which differ from those mentioned above in three main ways: First, our bounds on the algorithm's residual norms depend on the initial guess. Second, they give computable reduction factors for the residual norms for any nonsingular linear system and are applicable even to the singular case, if a certain condition is satisfied by the initial residual. Third, approximations to all factors in our bounds can be obtained during the GMRES run. These approximations lead to a heuristic which often allows us to predict after only a few steps, how GMRES will perform in later stages of the iteration. The paper is organized as follows: In Section 2 we introduce the GMRES algorithm and its mathematical properties. We then briefly review several convergence results in Section 3, before deriving new characterizations of GMRES-equivalent matrices in Section 4. Section 5 includes our new bounds for GMRES residual norms. In Section 6 we explain how to obtain approximations to the factors in our bounds from information generated during the GMRES run. We also devise heuristics for the behavior of these approximations and for the prediction of the performance of the GMRES algorithm. Section 7 includes numerical examples, and Section 8 contains our concluding remarks.

We point out that the linear system (1.1) might be singular, if not assumed otherwise. Throughout this paper, we assume that all calculations are performed in exact arithmetic. We let π_n denote the set of polynomials of degree at most n with value one at the origin. Furthermore, $\|\cdot\|$ denotes the Euclidean vector and corresponding matrix norm. By $\Lambda(M)$ we denote the spectrum and by M^H the Hermitian transpose of the matrix $M \in \mathbf{C}^{N\times N}$, respectively. If M is nonsingular, we define $\kappa(M) := \|M\|\|M^{-1}\|$, and $\kappa(M) := \infty$, otherwise. For $n = 1, 2, \ldots$, we define $K_n(M, v) := \text{span}\{v, Mv, \ldots, M^{n-1}v\}$, the nth Krylov space generated by the matrix M and the vector $v \in \mathbf{C}^N$. For technical reasons we also define $K_0(A, v) := \{0\}$.

2 The mathematical properties of GMRES

In this section we introduce the GMRES algorithm and state several of its properties. We are not concerned with implementational details.

Definition 2.1 *Suppose that x_0 is an initial guess for the solution of a linear system (1.1) and define the initial residual $r_0 := b - Ax_0$. For $n = 1, 2, \ldots$, let*

$$x_n \in x_0 + K_n(A, r_0) \tag{2.1}$$

be a vector, such that

$$r_n := b - Ax_n \in r_0 + AK_n(A, r_0) \tag{2.2}$$

satisfies

$$\|r_n\| = \min_{r \in r_0 + AK_n(A, r_0)} \|r\|, \tag{2.3}$$

then the vectors x_n and r_n are called nth GMRES iterate and residual, respectively.

As a comparison with [22, Formulas (4) and (8)] shows, our definition of the GMRES iterates and residuals is mathematically equivalent to their original derivation by Saad and Schultz. The next well known result (see e.g. [5, p. 8]) justifies Definition 2.1.

Lemma 2.2 *Suppose that $A \in \mathbf{C}^{N\times N}$ and $r_0 \in \mathbf{C}^N$. Then for every $n = 1, 2, \ldots$, there exists a unique vector $r_n \in r_0 + AK_n(A, r_0)$ that satisfies (2.3).*

Thus, for $n = 1, 2, \ldots$, the GMRES residuals are uniquely defined. In case of a nonsingular linear system, uniqueness of the residuals results in uniqueness of the iterates. Definition 2.1 leads to the following algorithm, which does not require uniqueness of the iterates.