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SOME REMARKS ON THE RESTARTED AND AUGMENTED GMRES METHOD*

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Abstract. Starting from the residual estimates for GMRES formulated by many authors, usually in terms of the quotient of the Hermitian part and the norm of a matrix or by using the field of values of a matrix, we present more general estimates which hold also for restarted and augmented GMRES. Sufficient conditions for convergence are formulated. All estimates are independent on the choice of an initial approximation.

Key words. Linear equations, restarted and augmented GMRES method, residual bounds, non-stagnation conditions.

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1. Introduction. Let us consider the GMRES algorithm [15] for solution of a non-singular and non-Hermitian system

$$Ax = b, \quad A \in \mathbb{C}^{n\times n}, \quad x, b \in \mathbb{C}^n. \tag{1.1}$$

Let x_0 be an initial approximation, $r_0 = b - Ax_0 \neq 0$ the residual,

$$K_m = [r_0, Ar_0, \ldots, A^{m-1}r_0]$$

the Krylov matrix and $\mathcal{K}_m(A, r_0) = \mathrm{Range}(K_m)$ the Krylov subspace. The GMRES algorithm constructs the new approximation x_m in the affine space $x_0 + \mathcal{K}_m(A, r_0)$ such that

$$r_m = b - Ax_m \perp \mathrm{Range}(AK_m).$$

In contrast to systems with normal matrices, eigenvalue distributions do not necessarily determine the speed of convergence. It can happen, in the extreme case, that

$$\|r_0\| = \|r_1\| = \cdots = \|r_{n-1}\| > 0 \quad \text{and} \quad \|r_n\| = 0$$

for an arbitrary spectrum, if exact arithmetic is used; for more information, see [1, 13]. In spite of this pessimistic information, the GMRES method is one of the most popular iterative methods, and various estimates for $\|r_m\|$ are studied. Experience shows that the convergence is often superlinear, while many bounds indicate only linear convergence. These bounds do not characterize the behaviour of $\|r_m\|/\|r_0\|$, and they can be misleading for highly non-normal matrices. Bounds for GMRES are based on eigenvalues, or on the field of values (or pseudospectra), and a discussion on how descriptive these bounds are, can be found in [10]. Usual estimates have the form

$$\|r_m\|^2 \leq (1 - \varrho)^m \|r_0\|^2, \tag{1.2}$$

where $\varrho \in (0, 1]$; see [2, 4, 7, 9, 11, 18]. The bounds of the form (1.2) ensure convergence of GMRES(m). It is well known (see [9]) that if the matrix $H = (A + A^H)/2$ is positive definite, then $\varrho = (\lambda_{\min}(H)/\|A\|)^2$, and the inequality $0 < \varrho \leq 1$ holds. The inequality (1.2) is proved for a larger class of matrices in [17]. A non-stable situation appears if the number ϱ is near zero. This difficulty can be caused by the presence of eigenvalues close

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to zero (see [12]) as this slows down the convergence of GMRES, especially during the first iterations, and a restarted version may stagnate. There are many papers [3, 5, 6, 8, 14, 16] addressing the question of how to remedy stagnation. The procedure GMRES(m,k), proposed by Morgan [14], will be considered in this paper, i.e., the restarted GMRES with restart m, where a subspace of dimension k is added to the subspace $\mathcal{K}_m(A,r_0)$. The residual vector of the GMRES(m,k) method will be denoted by r_s, where $s=m+k$ is the dimension of the augmented space. In this paper, new estimates for $\|r_s\|$ generalize the results from [11] and [19], and give new sufficient conditions for convergence of GMRES.

In Section 2, the first restarted run of GMRES(m,k) is considered, and interesting conclusions for the GMRES method are discussed. In Section 3, the GMRES(m,k) algorithm is briefly analysed. In Section 4, new upper bounds for the residual norm are derived and the convergence of GMRES(m,k) is studied. Remarks and open problems are discussed in the concluding section.

Let $s=m+k$, and let $r_0^{(j)}$ and $r_s^{(j)}$ denote the initial and resultant residual vector after the jth restart, respectively. The upper index will be omitted if it will be evident from the context that both vectors are considered for the same restart. Throughout the paper we put $v=r_0/\|r_0\|$. Considering the GMRES(m,k) method, let a space $\mathrm{Range}(Y_k)$ of dimension k be added to $\mathcal{K}_m(A,r_0)$, where $Y_k\in\mathbb{C}^{n\times k}$.

The symbol S_n denotes the unit sphere in $\mathbb{C}^n$, and $\|\cdot\|$ is the Euclidean norm. The symbol $\mathcal{P}_s^0$ denotes all polynomials of degree at most s which take the value zero at the origin. We will assume that all considered Krylov and augmented Krylov subspaces have maximal dimension. The symbol $W(B)$ denotes the field of values of the matrix $B\in\mathbb{C}^{n\times n}$. Exact arithmetic is assumed throughout the paper.

2. The first restarted run of GMRES(m,k), and conclusions for GMRES(s). If we carry out the GMRES(m,k) process, we basically perform the GMRES algorithm with the space $\mathcal{K}_m(A,r_0)+\mathrm{Range}(Y_k)$, instead of $\mathcal{K}_m(A,r_0)$; for more details, see [19] and [14].

In the first restart we usually put $Y_k=[A^m r_0, A^{m+1}r_0,\ldots,A^{m+k-1}r_0]$. Hence the estimate for $\|r_s^{(1)}\|^2/\|r_0\|^2$ is equivalent with the estimate for GMRES(s). The approximation $x_s\in x_0+\mathcal{K}_s(A,r_0)$ is constructed such that $r_s=b-Ax_s\perp A\mathcal{K}_s(A,r_0)$. The residual vector r_s can be expressed in the form $r_s=\|r_0\|(v-q_s(A)v)$, where $q_s\in\mathcal{P}_s^0$ fulfills the condition

$$q_s=\arg\min_{q\in\mathcal{P}_s^0}\|v-q(A)v\|.$$

An easy calculation yields, for every $q\in\mathcal{P}_s^0$, the relations

$$\begin{aligned}\frac{\|r_s\|^2}{\|r_0\|^2}&=1-\frac{|v^Hq_s(A)v|^2}{\|q_s(A)v\|^2}\le 1-\min_{w\in S_n}\frac{|w^Hq(A)w|^2}{\|q(A)\|^2}\\&=1-\min_{w\in S_n}\frac{|w^HH_qw|^2+|w^HS_qw|^2}{\|q(A)\|^2},\end{aligned}\tag{2.1}$$

where the matrices H_q and $\boldsymbol{i}S_q$ denote the Hermitian and skew-Hermitian part of the matrix $q(A)$ respectively. Here $\boldsymbol{i}$ denotes the imaginary unit; for a detailed computation, see [11, 19]. We have the following result, formulated in the real case for GMRES in Grcar's report [11, Corollary to Theorem 1].

THEOREM 2.1. *Let $s\in\{1,2,\ldots,n-1\}$. If a polynomial q of degree s with $q(0)=0$ exists such that*

$$\min_{w\in S_n}|w^HH_qw|>0\quad\textit{or}\quad\min_{w\in S_n}|w^HS_qw|>0,\tag{2.2}$$

then GMRES(s) is convergent, i.e., the iterations converge to the unique solution of (1.1).

Proof. If the assumption of Theorem 2.1 is fulfilled, then in each restart we obtain for the quotient $\|r_s\|^2/\|r_0\|^2$ the estimate $\|r_s\|^2/\|r_0\|^2 < 1-\varrho$, where $1-\varrho \in (0,1)$, according to (2.1). Hence

$$\|r_s^{(j)}\|^2 \leq (1-\varrho)\|r_0^{(j)}\|^2 = (1-\varrho)\|r_s^{(j-1)}\|^2 \leq \cdots \leq (1-\varrho)^j\|r_0\|^2,$$

and therefore $\lim_{j\to\infty} r_s^{(j)} = 0$. ◻

REMARK 2.2. The estimate for $r_s^{(j)}$ does not describe, in general, the real progress of the residual vector.

REMARK 2.3. If H_q is positive or negative definite, then the first inequality in (2.2) holds. The same can be analogously said for S_q. Often in the literature the expression "the matrix H_q or S_q is positive or negative definite" is used to refer to the condition (2.2).

For arbitrary $x \in S_n$ and $q \in \mathcal{P}_s^0$ there holds

$$x^H q^2(A)x = x^H(H_q + \boldsymbol{i}S_q)^2 x = \|H_q x\|^2 - \|S_q x\|^2 + 2\boldsymbol{i}\,\mathrm{Re}(x^H H_q S_q x). \tag{2.3}$$

If

$$\|H_q x\| < \|S_q x\| \quad \text{or} \quad \|H_q x\| > \|S_q x\|, \quad \forall x \in \mathbb{C}^n,\ x \neq 0, \tag{2.4}$$

then, according to (2.3), $\mathrm{Re}(x^H q^2(A)x) < 0$, $\forall x \neq 0$, or $\mathrm{Re}(x^H q^2(A)x) > 0$, $\forall x \neq 0$, respectively, and $W(q^2(A))$ does not contain 0. Therefore, GMRES(j) is convergent for all $j \geq 2s$, according to the results in [7, 10, 18].

Let us consider the first inequality in (2.4). If S_q is nonsingular, then the first inequality in (2.4) is equivalent to the following

$$\left\{\frac{\|H_q S_q^{-1} S_q x\|}{\|S_q x\|} < 1, \forall x \in \mathbb{C}^n \setminus \{0\}\right\} \Leftrightarrow \left\{\sup_{x\neq 0} \frac{\|H_q S_q^{-1}(S_q x)\|}{\|(S_q x)\|} < 1\right\} \Leftrightarrow \|H_q S_q^{-1}\| < 1.$$

The strict inequalities follow from the continuity of the norm and the compactness of the unit sphere in finite dimensional spaces. Hence, $\|H_q S_q^{-1}\| < 1$ if and only if

$$\mathrm{Re}(x^H q^2(A)x) < 0, \quad \forall x \neq 0.$$

Analogously, if the matrix H_q is nonsingular, then $\|S_q H_q^{-1}\| < 1$ if and only if

$$\mathrm{Re}(x^H q^2(A)x) > 0, \quad \forall x \neq 0.$$

The concepts here formulated form another proof of the original result by Simoncini and Szyld [17], which is here generalized, to the complex case, for the matrix polynomial $q(A)$. Let us summarize the considerations above.

THEOREM 2.4. *Let $q \in \mathcal{P}_s^0$ be arbitrary. Let S_q or H_q be nonsingular. Then*

(a) *if S_q is nonsingular, then*

$$\left\{\mathrm{Re}(x^H q^2(A)x) < 0, \forall x \in \mathbb{C}^n, x \neq 0\right\} \quad \Leftrightarrow \quad \|H_q S_q^{-1}\| < 1;$$

(b) *if H_q is nonsingular, then*

$$\left\{\mathrm{Re}(x^H q^2(A)x) > 0, \forall x \in \mathbb{C}^n, x \neq 0\right\} \quad \Leftrightarrow \quad \|S_q H_q^{-1}\| < 1.$$

If $W(q(A)^2)$ does not contain 0, then GMRES(j) is convergent for all $j \geq 2s$.

3. The augmented GMRES method. Let some vector $y \in \mathbb{C}^n \setminus \{0\}$, be added to $\mathcal{K}_m(A, r_0)$. The iteration x_{m+1} is constructed in the linear variety

$$x_0 + \mathcal{K}_m(A, r_0) + \mathrm{span}\{y\};$$

see [14, 16, 19]. In this case $s = m+1$ and, analogously to the previous section, the residual vector r_{m+1} can be written in the form

$$r_{m+1} = \|r_0\|(v - q_m(A)v) - \beta_{m+1}Ay,$$

where the minimal residual condition $r_{m+1} \perp \mathrm{Range}(AK_m, Ay)$ determines $\beta_{m+1} \in \mathbb{C}$, as well as the coefficients of the polynomial $q_m \in \mathcal{P}_m^0$. Hence, for an arbitrary polynomial $q \in \mathcal{P}_m^0$ and $\beta \in \mathbb{C}$ we have

$$\|r_{m+1}\| \le \big\|\|r_0\|(v - q(A)v) - \beta Ay\big\| = \big\|\underbrace{\|r_0\|(I - q(A))}_{p(A)}v - A\hat{y}\big\|,$$

where $p(0) = \|r_0\|$ and $\hat{y} = \beta y$. The last relations yield the following theorem.

THEOREM 3.1. *Let $m \in \{1, 2, \ldots, n-1\}$ and p be a polynomial of degree at most m, $p(0) = \|r_0\|$. If the vector $\hat{y} \in \mathbb{C}^n$ which solves the equation*

$$A\hat{y} = p(A)v \tag{3.1}$$

is added to $\mathcal{K}_m(A, r_0)$, then $r_{m+1} = 0$.

A similar formulation is given by Saad in [16]. Unfortunately, solving equation (3.1) is a problem similar to the original one. We carry out another analysis.

4. The second and subsequent restarts. Let the subspace $\mathrm{Range}(Y_k)$ be added to $\mathcal{K}_m(A, r_0)$ in all following restarts, where $Y_k \in \mathbb{C}^{n \times k}$ and $m + k < n$. The matrix Y_k, and therefore $\mathrm{Range}(Y_k)$, is fixed here, and this is not the setting of most practical augmented subspace algorithms, where approximations to a "wanted" subspace (for example the eigenspace corresponding to the smallest eigenvalues) are calculated and updated during each restart. In many cases, a good approximation defined by a matrix Y_k is achieved after a small number of restarts, and used in the following restarts. In Section 2, we discussed the first restarted run of GMRES(m, k). During the next restarts, usually the eigenvalues and eigenvectors of the obtained Hessenberg matrix are used for the construction of a matrix Y_k, which is subsequently improved. There are many papers in which such techniques are described; see for example [3, 5, 6, 14]. Our goal is to describe in general the behaviour of the residual norm for GMRES(m, k).

Let us consider an arbitrary projection z of the vector $r_0 = \|r_0\|v$ onto the space $\mathrm{Range}(AK_m, AY_k)$. It can be written in the form $z = \|r_0\|q(A)v + Ay$, where $y \in \mathrm{Range}(Y_k)$ and $q \in \mathcal{P}_m^0$. Let $r = r_0 - z = \|r_0\|(v - q(A)v) - Ay$ and $U = [q(A)v, AY_k]$. It is assumed that U is full rank. The matrix $P = U(U^HU)^{-1}U^H$ is the orthogonal projector for the space $\mathrm{Range}(q(A)v, AY_k)$, and for the residual vector $r_s \perp \mathrm{Range}(AK_m, AY_k)$, there holds

$$\begin{aligned} \frac{\|r_s\|^2}{\|r_0\|^2} &\le 1 - v^HPv \le 1 - \|U^Hv\|^2 \lambda_{\min}((U^HU)^{-1}) \\ &\le 1 - \frac{\|U^Hv\|^2}{\lambda_{\max}(U^HU)} \le 1 - \frac{\|U^Hv\|^2}{\mathrm{Tr}(U^HU)} \\ &\le 1 - \min_{w \in S_n} \frac{|w^Hq(A)w|^2 + \|w^HAY_k\|^2}{\|q(A)\|^2 + \|AY_k\|_F^2}, \quad \forall\, q \in \mathcal{P}_m^0, \end{aligned} \tag{4.1}$$

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where $\lambda_{\min}((U^HU)^{-1})$ denotes the minimum eigenvalue of the matrix $(U^HU)^{-1}$, and $\|\cdot\|_F$ is the Frobenius norm.

Let the $(j-1)$th restart be performed. In the jth restart, the subspace $\mathrm{Range}(Y_k)$ is again added to $\mathcal{K}_m(A, r_0)$. We have in this case $r_0^{(j)} = r_s^{(j-1)}$, $v = r_0^{(j)}/\|r_0^{(j)}\|$, $v \perp \mathrm{Range}(AY_k)$, and

$$U^H v = \begin{bmatrix} (q(A)v)^H v \\ (AY_k)^H v \end{bmatrix} = \begin{bmatrix} (q(A)v)^H v \\ 0_{\ \dim k} \end{bmatrix} = ((q(A)v)^H v)e_1. \tag{4.2}$$

Hence,

$$\frac{\|r_s^{(j)}\|^2}{\|r_0^{(j)}\|^2} \leq 1 - |v^H q(A)v|^2 e_1^T (U^HU)^{-1} e_1. \tag{4.3}$$

Now, we estimate $e_1^T(U^HU)^{-1}e_1$ from the following inequalities:

$$\begin{aligned} 1 = (e_1^T e_1)^2 &= (e_1^T (U^HU)^{-\frac{1}{2}} (U^HU)^{\frac{1}{2}} e_1)^2 \\ &\leq \|(U^HU)^{-\frac{1}{2}} e_1\|^2 \, \|(U^HU)^{\frac{1}{2}} e_1\|^2 \\ &= (e_1^T (U^HU)^{-1} e_1)(e_1^T (U^HU) e_1), \end{aligned}$$

and, hence,

$$(e_1^T (U^HU)^{-1} e_1) \geq \frac{1}{e_1^T (U^HU) e_1} = \frac{1}{\|q(A)v\|^2}.$$

Substitution to (4.3) yields the estimate

$$\frac{\|r_s^{(j)}\|^2}{\|r_0^{(j)}\|^2} \leq 1 - \frac{|v^H q(A)v|^2}{\|q(A)v\|^2},$$

where $v \perp \mathrm{Range}(AY_k)$. Let us summarize all previous investigations and results in the following theorem.

THEOREM 4.1. *Let $m, k, s \in \{1, 2, \ldots, n-1\}$, $s = m + k < n$, and $Y_k \in \mathbb{C}^{n\times k}$ be a rank k matrix. Let the subspace $\mathrm{Range}(Y_k)$ be added to the corresponding Krylov subspace for all restarted runs. Let $j > 1$ be an integer. Then, for the jth restart and for all $q \in \mathcal{P}_m^0$, the following estimate holds*

$$\frac{\|r_s^{(j)}\|^2}{\|r_0^{(j)}\|^2} \leq 1 - \min_{\substack{w \in S_n \\ w \perp \mathrm{Range}(AY_k)}} \frac{|w^H q(A)w|^2}{\|q(A)\|^2}. \tag{4.4}$$

It follows immediately from (4.4) that if an integer m exists such that $m + k < n$ and the system of equations

$$w^H q(A) w = 0 \tag{4.5}$$
$$w^H A Y_k = 0 \tag{4.6}$$

does not have any solution on S_n (or equivalently has only the solution $w = 0$ in $\mathbb{C}^n$), then GMRES(m, k) is convergent.

REMARK 4.2. The same theorem can be formulated if the condition (4.5) is replaced either by the equality $w^H H_q w = 0$ or $w^H S_q w = 0$.

Let the equation (4.5) have a nontrivial solution, i.e., $0 \in W(q(A))$. Moreover let

$$M = \{u \in S_n | u^H q(A) u = 0\}.$$

The condition (4.6) suggests to find Y_k such that $u^H A Y_k = 0$ implies that $u \notin M$, and therefore to make the quotient in (4.1) less than 1. Let us remark that the last implication is equivalent with the relation

$$u \in M \quad \Rightarrow \quad u^H A Y_k \neq 0, \tag{4.7}$$

which may be easier to verify.

REMARK 4.3. If $\mathrm{Range}(Y_k)$ is an A-invariant subspace, then the product AY_k in the relations (4.2), (4.4), (4.6), and (4.7) can be substituted by Y_k.

In [19] we find an estimate for the case when the space $\mathrm{Range}(\tilde{Y}_k)$ is added to the Krylov subspace, and the gap between $\mathrm{Range}(\tilde{Y}_k)$ and an A-invariant space $\mathrm{Range}(Y_k)$ is less than some small number ε. The estimate is similar to (4.4), only the set for the minimum is larger and depends on ε.

5. Conclusions and some open questions. Restarting tends to slow down convergence, and the difficulty may be caused by the eigenvalues closest to zero. These are potentially bad, because it is impossible to have a polynomial p of degree m such that $p(0) = 1$ and $|p(z)| < 1$ on any Jordan curve around the origin; see [12, p. 55]. Usually, an eigenspace corresponding to the smallest eigenvalues is taken for $\mathrm{Range}(Y_k)$, and the corresponding algorithms give good results [14, 16]. If we consider a normal matrix A with the eigenvalues having only positive or negative real part and $q(z) = z$, then $W(A)$ is the convex hull of the spectrum of A. If the Krylov subspace is enriched by an eigenspace corresponding to the smallest eigenvalues, and these eigenvalues are therefore removed from the spectrum, then the convex hull of the remaining eigenvalues can be far from zero and, consequently, the right hand side of (4.4) is smaller and the estimate is better. When an eigenspace corresponding to the smallest eigenvalues is added to the Krylov space, the convergence is faster and stagnation is removed in practical computation.

In our theoretical considerations, an arbitrary subspace was considered, and the question "to find some sufficient condition for convergence" was transformed into the question whether the intersection of fields of values and sets of the form (4.6) contains zero or not. The above investigations imply some open problems.

1) How to estimate generally, for a given polynomial q, all solutions of the equation $w^H q(A) w = 0$, for $w \in S_n$, with the constraint $w \perp \mathrm{Range}(AY_k)$, and vice versa how to construct the polynomial q fulfilling the assumption of Theorem 4.1?
2) How to obtain, for special matrices and polynomials, the behaviour of the integer function

$$f(j) = 1 - \min_{\substack{w \in S_n \\ w \perp \mathrm{Range}(AY_k)}} \frac{|w^H q_j(A) w|^2}{\|q_j(A)\|^2}, \quad j \in [1, s],$$

and compare $f(j)$ with the behaviour of the sequence $\|r_j\|^2/\|r_0\|^2$, for j between 1 and the index of the restart? (This would be the answer on the question on how descriptive these bounds are.)
3) How to find an inexact solution of (3.1) very fast?

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