

ON THE ADMISSIBLE CONVERGENCE CURVES FOR RESTARTED GMRES

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Abstract. This paper studies admissible convergence curves for restarted GMRES and their relation to the curves for full GMRES. It shows that stagnation at the end of a restart cycle is mirrored at the beginning of the next cycle. Otherwise, any non-increasing convergence curve is possible and pairs $\{A, b\}$ are constructed such that when restarted GMRES is applied to $Ax = b$, prescribed residual norms and Ritz values for the individual cycles are generated. Additionally, A can have any spectrum. The constructed systems lead to full GMRES processes that can be generated with short recurrences and offer some insight into the phenomenon of larger restart lengths being able to result in slower convergence.

Key words. restarted GMRES, Arnoldi process, GMRES stagnation, prescribed convergence, short recurrence GMRES

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1. Introduction. Krylov subspace methods are popular for the solution of linear systems

$$Ax = b, \quad A \in \mathbb{C}^{n \times n}, b \in \mathbb{C}^n \quad (1.1)$$

with non-singular, sparse and possibly very large matrices A . If A is non-Hermitian, one can use methods like Bi-CG [16], QMR [17] or Bi-CGSTAB [31] based on short recurrences to build the underlying Krylov subspaces. They require limited storage and computational costs per iteration, but convergence curves for the residual norms can oscillate and the methods can break down before the solution has been found (in exact arithmetics). In the GMRES method [27], the k th iterate x_k minimizes the norm of the residual vector $r_k = b - Ax_k$ over all vectors in the k th Krylov subspace $\text{span}\{r_0, Ar_0, \dots, A^{k-1}r_0\}$, leading to non-increasing residual norms. The minimization property can also be formulated as

$$\|r_k\| = \min_{p \in \pi_k} \|p(A)r_0\|, \quad (1.2)$$

where π_k is the set of polynomials of degree k with the value one at the origin; $\|\cdot\|$ denotes the Euclidean norm for vectors and the induced norm for matrices. The employed basis for the k th Krylov subspace being orthogonal in GMRES, it must be generated with long recurrences. Storage and computational costs to find the solution of the minimization problem (1.2) therefore grow with the iteration number k . As a consequence, the GMRES method in practice almost always needs to be restarted: After a small number of m iterations, the current approximation x_m is used as the initial approximation for a new series of m GMRES iterations and this process is repeated. We will denote it by GMRES(m) and will call the non-restarted process full GMRES. GMRES(m) produces non-increasing residual norms just as full GMRES, but there is no guarantee that the solution of (1.1) has been found by the n th iteration. In fact, there is no guarantee that the solution will be found at all, as iterates may stagnate. In that case, GMRES(m) produces identical approximations during an entire cycle of m iterations and consequently, all subsequent cycles behave the same way.

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Part of the available convergence results for GMRES(m) consider non-stagnation conditions (see, e.g., [11, 26, 35, 30, 36]) and a large number of techniques has been proposed to reduce the risk of stagnation. Especially strategies using approximate eigenspaces to deflate the matrix or augment the Krylov subspaces have been successful (see, e.g., [10], [26], [4], [19]). In this paper we do not consider such strategies but restrict to the analysis of the restarted GMRES process described in the previous paragraph, which is already complicated by itself. Some results of convergence analysis for full GMRES (which is not straightforward either) can be inherited, but other issues are specific for restarting. For example, linear systems have been encountered where the speed of convergence seems to be *inversely* proportional to the restart length, i.e. a larger m yields slower convergence of GMRES(m), see, e.g. [12], [10]. A sound explanation for this phenomenon is missing. Detailed investigations of the restart mechanism and its consequences for convergence behavior can be found, among others, in [5],[29], [34] and [32].

One approach to convergence analysis is to study the form of the matrices (and right-hand sides) that generate a particular convergence curve, see e.g. [1] and [22, Section 5.7.4] for full GMRES. A classical theorem by Greenbaum, Pták and Strakoš is that any non-increasing convergence curve can be generated by full GMRES with matrices having prescribed (nonzero) eigenvalues [21], [20], [22]. This shows that eigenvalues alone are in general not sufficient to describe convergence behavior (see also [23]).

The same approach to convergence analysis was applied to GMRES(m) by Vecharynski and Langou [33] and Schweitzer [28] considers the restarted FOM method. This paper can be seen as an extension of the results in [33], which focus on so-called cycle-convergence. More precisely, [33] prescribes the residual norms for the last (m th) iterate of every restart cycle. We will concentrate on the residual norms *inside* cycles through the construction of linear systems that generate in every cycle Hessenberg matrices with prescribed entries. As a by-product, we can prescribe the Ritz values of restart cycles. In [33] it is assumed that at the end of every cycle, there is a strict decrease of the residual norm for the m th iterate in comparison with the previous iteration. We will show that the case where stagnation is allowed at the end of a cycle has consequences for the behavior in the next cycle and that it leads to an interesting characterization of inadmissible convergence curves for GMRES(m). We also address the relation of the possible convergence curves with the residual norms that can be generated by full GMRES applied to the same system. Finally, we offer some insight into how it is possible that the speed of convergence can be inversely proportional to the restart length.

The paper is organized as follows. In the remainder of this section we introduce some notation and recall relevant results related to full GMRES. The second section describes inadmissible convergence curves for GMRES(m) and the next section constructs linear systems generating any admissible curve with prescribed spectrum for the system matrix and prescribed Ritz values in the individual restart cycles. Section 4 shows that the constructed systems allow the full GMRES process to be carried out with short recurrences and that they lead to the counterintuitive situation described above where with $m' > m$, GMRES(m') yields slower convergence than GMRES(m). Further comments and conclusions are given in Section 5. Throughout the paper we assume exact arithmetics and we assume that the initial guess x_0 in (restarted) GMRES processes is zero. With “the subdiagonal” and “subdiagonal entries” we will mean the (entries on the) first diagonal under the main diagonal. We will denote by e_j the j th column of the identity matrix of appropriate order.

1.1. Notation and preliminaries. We consider in total not more than $N - 1$ restarts where $Nm < n$. In words, the total number of GMRES iterations inside all cycles (including the initial cycle) is smaller than the system size. This does not represent a restriction for most practical situations. We will attempt to construct matrices A and right-hand sides b such that if GMRES(m) is applied, it exhibits some prescribed behavior for the residual norms and possibly

the Ritz values. A and b are always constructed as

$$A = HVV^*, \quad b/\|b\| = Ve_1, \quad (1.3)$$

for an upper Hessenberg matrix H and a unitary matrix V . For the purposes of this paper it suffices to restrict to unreduced Hessenberg matrices H . Note that (1.3) does not in general represent the Arnoldi decomposition resulting from applying the Arnoldi orthogonalization process to A and b , because we do not require the subdiagonal entries of H to be real positive.

GMRES residual norms are unitarily invariant, i.e. GMRES applied to B and c gives the same residual norms as GMRES applied to WBW^* and Wc for any unitary matrix W . With respect to (1.3) this means that it suffices to study GMRES for H with right-hand side e_1 . The same holds for the Ritz values obtained from the Arnoldi process. To construct matrices and right-hand sides yielding prescribed residual norms and Ritz values, we will therefore concentrate in (1.3) on the choice of H and consider V a free parameter matrix.

Any product of the form UCU^{-1} where U is nonsingular upper triangular and C is a companion matrix yields an unreduced upper Hessenberg matrix. Reversely, any unreduced upper Hessenberg matrix H can be decomposed as

$$H = UCU^{-1}, \quad (1.4)$$

where U is nonsingular upper triangular and C is the companion matrix for the polynomial whose roots are the eigenvalues of H . To find U , it suffices to equate consecutively the columns 1 till $n-1$ of the equation $HU = UC$ starting with Ue_1 being a nonzero multiple of e_1 . The decomposition (1.4) is useful for creating Hessenberg matrices with a given spectrum yielding prescribed residual norms and Ritz values when GMRES is applied with right-hand side e_1 . The next theorem shows that in *full* GMRES, the choice of the first row of U^{-1} can force prescribed residual norms and the columns of U^{-1} determine Ritz values. It is a slight modification of [8, Theorem 1], formulated in terms of the Hessenberg matrix that is actually generated by GMRES.

THEOREM 1.1. *Consider a set of tuples of complex numbers*

$$\begin{aligned} \mathcal{R} = \{ & \rho_1^{(1)}, \\ & (\rho_1^{(2)}, \rho_2^{(2)}), \\ & \vdots \\ & (\rho_1^{(n-1)}, \dots, \rho_{n-1}^{(n-1)}), \\ & (\lambda_1, \dots, \lambda_n) \}, \end{aligned}$$

such that $(\lambda_1, \dots, \lambda_n)$ contains no zero number and consider n positive numbers

$$f(0) \geq f(1) \geq \dots \geq f(n-1) > 0,$$

such that for $i = 1, \dots, n-1$, $f(i-1) = f(i)$ if and only if $(\rho_1^{(i)}, \dots, \rho_i^{(i)})$ contains a zero number.

If A is a matrix of order n and b a nonzero n -dimensional vector, then the following assertions are equivalent:

1. *The GMRES method applied to A and right-hand side b with zero initial guess yields residual vectors r_i , $i = 0, \dots, n-1$ such that*

$$\|r_i\| = f(i), \quad i = 0, \dots, n-1,$$

A has eigenvalues $\lambda_1, \dots, \lambda_n$ and $\rho_1^{(i)}, \dots, \rho_i^{(i)}$ are the eigenvalues of the i th leading principal submatrix of the generated Hessenberg matrix (the Ritz values) for all $i = 1, \dots, n-1$.

2. The GMRES method applied to A and right-hand side b with zero initial guess generates an upper Hessenberg matrix of the form

$$H = \begin{bmatrix} \chi^T \\ 0 & \Sigma \end{bmatrix}^{-1} C^{(n)} \begin{bmatrix} \chi^T \\ 0 & \Sigma \end{bmatrix},$$

where $C^{(n)}$ is the companion matrix of the polynomial with roots $\lambda_1, \dots, \lambda_n$,

$$\chi_0 = \frac{1}{f(0)}, \quad |\chi_i| = \sqrt{\frac{1}{f(i)^2} - \frac{1}{f(i-1)^2}}, \quad i = 1, \dots, n-1$$

and the entries of the nonsingular upper triangular matrix Σ of size $n-1$ satisfy

$$\prod_{j=1}^i (\rho - \rho_j^{(i)}) = \frac{1}{\sigma_{i,i}} \left(\chi_i + \sum_{j=1}^i \sigma_{j,i} \rho^j \right), \quad \sigma_{i,i} \in \mathbb{R}, \quad \sigma_{i,i} > 0, \quad i = 1, \dots, n-1.$$

Proof. It is easily seen from equating consecutively the columns 1 till $n-1$ of the equation $HU = UC$ that H has real positive subdiagonal if and only if U^{-1} has real positive main diagonal. Thus the matrix H in the second assertion has real positive subdiagonal and can be generated by an Arnoldi process performed in GMRES. Assume the second assertion of [8, Theorem 1] holds for $k = n$. One can always find a unitary diagonal scaling matrix D_1 such that the main diagonal of

$$\begin{bmatrix} & g^T \\ 0 & T_{n-1} \end{bmatrix} D_1$$

is real positive. Then the unitary matrix V can be replaced with the unitary matrix VD_1^* . If the second assertion of the present theorem holds, then one can find a unitary diagonal scaling matrix D_2 such that $\chi^T D_2$ is real positive. \square

Because the matrix U^{-1} in the decomposition (1.4) of a generated upper Hessenberg matrix determines both residual norms and Ritz values, it would be nice to have a formula to compute U^{-1} directly from H , without knowing U .

PROPOSITION 1.2. *Let $H = UCU^{-1}$ be the decomposition (1.4) and let $\nu_{i,j}$ be the entries of U^{-1} . Then*

$$\begin{bmatrix} \nu_{1,i+1} \\ \vdots \\ \nu_{i+1,i+1} \end{bmatrix} = \frac{1}{h_{i+1,i}} \left(\begin{bmatrix} 0 \\ \nu_{1,i} \\ \vdots \\ \nu_{i,i} \end{bmatrix} - \begin{bmatrix} U_i^{-1} h_i \\ \vdots \\ 0 \end{bmatrix} \right), \quad i = 1, \dots, n-1, \quad (1.5)$$

where $h_i = [h_{1,i}, \dots, h_{i,i}]^T$ and where U_i is the leading principal submatrix of size i of U .

Proof. See [24, Section 4]. \square

This gives a recursive formula for the entries of the first row of U^{-1} , which determine the generated GMRES residual norms.

LEMMA 1.3. *Let GMRES generate the Hessenberg matrix H and consider the recursion*

$$\chi_0 = \frac{1}{\|r_0\|}, \quad \chi_i = \frac{-1}{h_{i+1,i}} [\chi_0, \dots, \chi_{i-1}]^T \begin{bmatrix} h_{1,i} \\ \vdots \\ h_{i,i} \end{bmatrix}, \quad i = 1, 2, \dots, n-1. \quad (1.6)$$

Then $\chi = [\chi_0, \dots, \chi_{n-1}]^T$ is the first row of U^{-1} in the decomposition (1.4) of H (with $Ue_1 = \|r_0\|e_1$), and the i th residual norm satisfies

$$\|r_i\|^2 = \left(\sum_{j=0}^i |\chi_j|^2 \right)^{-1}, \quad i = 1, 2, \dots, n-1. \quad (1.7)$$

Proof. The fact that the first row of U^{-1} satisfies the recursion follows from equating the first row in (1.5). Because of Theorem 1.1, the residual norms satisfy

$$\frac{1}{\|r_0\|} = |\chi_0|, \quad \sqrt{\frac{1}{\|r_i\|^2} - \frac{1}{\|r_{i-1}\|^2}} = |\chi_i|, \quad i = 1, \dots, n-1.$$

Equality (1.7) follows from a straightforward induction argument applied to $\frac{1}{\|r_i\|^2} - \frac{1}{\|r_{i-1}\|^2} = |\chi_i|^2$, $i = 1, \dots, n-1$. \square

Formula (1.7) is most probably not as stable as the usual way to compute GMRES residual norms based on a QR-decomposition of the generated Hessenberg matrix, but it will prove to be useful in Section 4.

As mentioned before, all relevant values in GMRES are obtained from the Hessenberg matrix and this clearly also holds for the size $(m+1) \times m$ upper Hessenberg matrix generated in some cycle of GMRES(m). In the whole paper we will therefore focus on the choices of the small Hessenberg matrices of the individual restart cycles. In fact, we will attempt to prescribe all their entries. Because of its importance for the further development, we give the formula for creating the desired small Hessenberg matrices explicitly in a new corollary (though it is a straightforward consequence of Theorem 1.1).

COROLLARY 1.4. *Consider a set of tuples of complex numbers*

$$\mathcal{R} = \left\{ \begin{aligned} &\rho_1^{(1)}, \\ &(\rho_1^{(2)}, \rho_2^{(2)}), \\ &\vdots \\ &(\rho_1^{(m-1)}, \dots, \rho_{m-1}^{(m-1)}), \\ &(\rho_1^{(m)}, \dots, \rho_m^{(m)}) \end{aligned} \right\},$$

and $m+1$ positive numbers

$$f(0) \geq f(1) \geq \dots \geq f(m-1) \geq f(m) > 0,$$

such that for $i = 1, \dots, m$, $f(i-1) = f(i)$ if and only if $(\rho_1^{(i)}, \dots, \rho_i^{(i)})$ contains a zero number. Consider GMRES applied to a non-singular matrix of size n and an n -dimensional vector, where $n \geq m$. The following assertions are equivalent:

1. The residual vectors generated by m iterations of GMRES satisfy

$$\|r_i\| = f(i), \quad i = 0, \dots, m$$

and the generated Ritz values are $(\rho_1^{(i)}, \dots, \rho_i^{(i)})$ after the i th iteration for all $i = 1, \dots, m$.

2. The Hessenberg matrix generated after m iterations is of the form

$$\hat{H}_m = \begin{bmatrix} \chi_0 & \cdots & \chi_m \\ & 0 & \Sigma_m \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ I_m \end{bmatrix} \begin{bmatrix} \chi_0 & \cdots & \chi_{m-1} \\ & 0 & \Sigma_{m-1} \end{bmatrix} \in \mathbb{C}^{(m+1) \times m} \quad (1.8)$$

where

$$\chi_0 = \frac{1}{f(0)}, \quad |\chi_i| = \sqrt{\frac{1}{f(i)^2} - \frac{1}{f(i-1)^2}}, \quad i = 1, \dots, m. \quad (1.9)$$

and Σ_m is a nonsingular upper triangular matrix of size m with leading principal submatrix Σ_{m-1} of size $m-1$ whose entries satisfy

$$\prod_{j=1}^i (\rho - \rho_j^{(i)}) = \frac{1}{\sigma_{i,i}} \left(\chi_i + \sum_{j=1}^i \sigma_{j,i} \rho^j \right), \quad \sigma_{i,i} \in \mathbb{R}, \quad \sigma_{i,i} > 0, \quad i = 1, \dots, m.$$

2. Inadmissible convergence curves. In this section we investigate whether, as is the case for full GMRES, any non-increasing convergence curve is possible for restarted GMRES. We will see that the answer is negative and describe some inadmissible convergence curves. To this end, we study the restrictions that the Hessenberg matrix from a given cycle puts on the Hessenberg matrix for the next restart cycle. For ease of exposition, we will start by comparing the initial cycle with the second cycle (the first restart cycle) and then generalize for the other cycles (without proof if the generalization is straightforward).

Let the residual vectors generated in the first two cycles of GMRES(m) be denoted as

$$r_0^{(1)} = b, r_1^{(1)}, \dots, r_m^{(1)}, \quad r_0^{(2)} = r_m^{(1)}, r_1^{(2)}, \dots, r_m^{(2)}.$$

We wish to construct A and b of the form (1.3) such that in the m iterations of the initial cycle the generated Arnoldi decomposition is

$$AV_m^{(1)} = V_{m+1}^{(1)} \hat{H}_m^{(1)}, \quad \text{where} \quad V_{m+1}^{(1)*} V_{m+1}^{(1)} = I_{m+1}, \quad V_{m+1}^{(1)} e_1 = b/\|b\|. \quad (2.1)$$

Here the upper Hessenberg matrix $\hat{H}_m^{(1)}$ of size $(m+1) \times m$ is a *given* matrix whose entries have been chosen such that prescribed residual norms and Ritz values are obtained. This can be done with Corollary 1.4. $V_{m+1}^{(1)}$ is an arbitrary matrix of size $n \times (m+1)$ with orthonormal columns. Because no restart took place in the initial cycle, it is trivial that we can choose the first m columns of H and the first $m+1$ columns v_1, \dots, v_{m+1} of V in (1.3) as

$$H \begin{bmatrix} I_m \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{H}_m^{(1)} \\ 0 \end{bmatrix}, \quad V \begin{bmatrix} I_{m+1} \\ 0 \end{bmatrix} = [v_1, \dots, v_{m+1}] = V_{m+1}^{(1)}. \quad (2.2)$$

At the beginning of the restart, the new initial Arnoldi vector is the normalized last residual vector of the previous (first) cycle and can be written as a linear combination of the Arnoldi vectors of the previous (first) cycle. It is not difficult to see that the coefficients of this linear combination are given by the entries of the normalized vector $e_1 - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger e_1$, where B^\dagger denotes the Moore-Penrose pseudoinverse of a matrix B . What is more interesting is that these entries are given by the numbers χ_0, \dots, χ_m which depend only on the residual norms of the initial cycle (except for the phase angles), see (1.9).

LEMMA 2.1. *Let GMRES generate in its m th iteration Arnoldi vectors v_1, \dots, v_{m+1} and an upper Hessenberg matrix $\hat{H}_m^{(1)}$ with decomposition (1.8), i.e.*

$$\frac{1}{\|r_0\|} = |\chi_0|, \quad \sqrt{\frac{1}{\|r_i\|^2} - \frac{1}{\|r_{i-1}\|^2}} = |\chi_i|, \quad i = 1, \dots, m.$$

If

$$\gamma^{(1)} = \|r_m^{(1)}\| \begin{bmatrix} \bar{\chi}_0 \\ \vdots \\ \bar{\chi}_m \end{bmatrix} \in \mathbb{C}^{m+1}, \quad (2.3)$$

where $\bar{\alpha}$ denotes the complex conjugate of a complex number α , then

$$(\gamma^{(1)})^* \hat{H}_m^{(1)} e_j = 0, \quad j = 1, \dots, m \quad (2.4)$$

and

$$\frac{r_m^{(1)}}{\|r_m^{(1)}\|} = [v_1, \dots, v_{m+1}] \gamma^{(1)}. \quad (2.5)$$

Proof. Because $\hat{H}_m^{(1)}$ has the form (1.8), we have

$$\|r_m^{(1)}\| e_1^T \begin{bmatrix} \chi_0 & \cdots & \chi_m \\ & 0 & \Sigma_m \end{bmatrix} \begin{bmatrix} \chi_0 & \cdots & \chi_m \\ & 0 & \Sigma_m \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ I_m \end{bmatrix} \begin{bmatrix} \chi_0 & \cdots & \chi_{m-1} \\ & 0 & \Sigma_{m-1} \end{bmatrix} = 0 \cdot e_1^T,$$

which proves (2.4). After m iterations of GMRES we have

$$r_m^{(1)} = V_{m+1}^{(1)} \left(\|r_0^{(1)}\| e_1 - \hat{H}_m^{(1)} y_m \right), \quad y_m = \arg \min \left\| \|r_0^{(1)}\| e_1 - \hat{H}_m^{(1)} y \right\|,$$

and with $y_m = \|r_0^{(1)}\| (H_m^{(1)})^\dagger e_1$, we have

$$r_m^{(1)} = \|r_0^{(1)}\| [v_1, \dots, v_{m+1}] \left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger \right) e_1.$$

Taking norms on both sides gives

$$\frac{\|r_m^{(1)}\|}{\|r_0^{(1)}\|} = \left\| \left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger \right) e_1 \right\|. \quad (2.6)$$

Thus

$$\frac{r_m^{(1)}}{\|r_m^{(1)}\|} = [v_1, \dots, v_{m+1}] c, \quad c = \frac{\left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger \right) e_1}{\left\| \left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger \right) e_1 \right\|}. \quad (2.7)$$

Furthermore,

$$(\gamma^{(1)})^* c = (\gamma^{(1)})^* \frac{\left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger \right) e_1}{\left\| \left(I_{m+1} - \hat{H}_m^{(1)} (\hat{H}_m^{(1)})^\dagger \right) e_1 \right\|} = \|r_m^{(1)}\| \frac{\chi_0}{\|r_m^{(1)}\|} \|r_0^{(1)}\| = 1,$$

where we used (2.7), (2.6) and (2.3). It is easily checked from (1.9), that $\|\gamma^{(1)}\| = 1$. By the Cauchy-Schwarz inequality $1 = (\gamma^{(1)})^* c \leq \|\gamma^{(1)}\| \|c\| = 1$, with equality if and only if $\gamma^{(1)}$ and c are collinear. \square

We wish to define further columns of H in (1.3) such that, for a *given* Hessenberg matrix $\hat{H}_m^{(2)}$, the Arnoldi decomposition build in the m iterations of the second cycle is

$$AV_m^{(2)} = V_{m+1}^{(2)} \hat{H}_m^{(2)}, \quad \text{where} \quad V_{m+1}^{(2)*} V_{m+1}^{(2)} = I_{m+1}, \quad V_{m+1}^{(2)} e_1 = V_{m+1}^{(1)} \gamma^{(1)}. \quad (2.8)$$

The Hessenberg matrix $\hat{H}_m^{(2)}$ is chosen such that it yields predefined residual norms and Ritz values for the second cycle (which can be achieved using Corollary 1.4); $V_{m+1}^{(2)}$ is an arbitrary matrix of size $n \times (m+1)$ with orthonormal columns.

The following lemma describes a relation between the Hessenberg matrices of the first two cycles $\hat{H}_m^{(1)}$, $\hat{H}_m^{(2)}$ and the Hessenberg matrix H in (1.3).

LEMMA 2.2. *Let GMRES applied to A and b of the form $A = VHV^*$, $b/\|b\| = Ve_1$ and satisfying (2.2), be restarted after m iterations with initial Arnoldi vector $[v_1, \dots, v_{m+1}] \gamma^{(1)}$. The restart cycle generates the Arnoldi decomposition (2.8) if and only if m iterations of the Arnoldi process with input matrix H and initial vector $[(\gamma^{(1)})^T \ 0]^T$ generate the decomposition*

$$HZ_m = Z_{m+1} \hat{H}_m^{(2)}, \quad \text{where} \quad Z_{m+1}^* Z_{m+1} = I_{m+1}, \quad Z_{m+1} e_1 = \begin{bmatrix} \gamma^{(1)} \\ 0 \end{bmatrix}. \quad (2.9)$$

Proof. It suffices to use $A = VHV^*$ and to define $Z_{m+1} \equiv V^* V_{m+1}^{(2)}$. \square

Lemma 2.2 says that the Hessenberg matrix $\hat{H}_m^{(2)}$ generated during the restart is fully determined by the vector $\gamma^{(1)}$ and by the Hessenberg matrix H in (1.3). Because the first m columns of H contain the Hessenberg matrix $\hat{H}_m^{(1)}$ generated during the initial cycle, $\hat{H}_m^{(2)}$ may be determined by $\hat{H}_m^{(1)}$, at least partially. This will depend upon the zeros in $\gamma^{(1)}$: if most of the trailing entries in $\gamma^{(1)}$ are zero, then most of the Arnoldi decomposition (2.9) lives on the first m columns of H and most of $\hat{H}_m^{(2)}$ is determined by $\hat{H}_m^{(1)}$.

LEMMA 2.3. *Let $j \geq 0$ be a nonnegative integer smaller than or equal to m . The j trailing entries of $\gamma^{(1)}$ are zero (i.e. $e_i^T \gamma^{(1)} \neq 0$, $i = 1, \dots, m+1-j$, $e_i^T \gamma^{(1)} = 0$, $i = m+2-j, \dots, m+1$) if and only if the last j iterations of the initial cycle stagnate, i.e.*

$$\|b\| \geq \|r_1^{(1)}\| \geq \dots \geq \|r_{m-j-1}^{(1)}\| > \|r_{m-j}^{(1)}\| = \dots = \|r_m^{(1)}\|.$$

Proof. This follows immediately from the definition of the entries of $\gamma^{(1)}$, see (2.3) and (1.9).

\square

We see that it is crucial for the ability to prescribe entries of $\hat{H}_m^{(2)}$ whether there is stagnation at the end of the initial cycle. Only if there is no stagnation, we have a chance that *all* entries of $\hat{H}_m^{(2)}$ can be prescribed; otherwise, some entries are predetermined by $\hat{H}_m^{(1)}$. In fact, it is the first columns that will be determined by $\hat{H}_m^{(1)}$:

LEMMA 2.4. *If for a nonnegative integer j smaller than or equal to m , the residual norms in the initial cycle satisfy*

$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \dots \geq \|r_{m-j-1}^{(1)}\| > \|r_{m-j}^{(1)}\| = \dots = \|r_m^{(1)}\|,$$

then the $(j+1) \times j$ left upper block $\hat{H}_{1,j}^{(2)}$ of the Hessenberg matrix $\hat{H}_m^{(2)}$ generated during the restart cycle is uniquely determined by the Hessenberg matrix $\hat{H}_m^{(1)}$ generated during the initial cycle.

Proof. The Hessenberg matrix $\hat{H}_m^{(2)}$ is the matrix generated by the Arnoldi decomposition (2.9), see Lemma 2.2. By Lemma 2.3, if we have j stagnating iterations at the end of the first cycle, the vector $\gamma^{(1)}$ in (2.9) is zero from position $m+2-j$ on. Therefore, when the Arnoldi decomposition (2.9) is computed, every next Arnoldi vector (i.e. every new column of Z_{m+1}) will have an additional position with nonzero entry beneath the nonzero entries of the previous Arnoldi vector. The first Arnoldi vector having a nonzero entry on position $m+1$ is $Z_{m+1}e_{j+1}$. Thus the first j columns of $\hat{H}_m^{(2)}$ are fully determined by the first m columns of H and by $\gamma^{(1)}$ which both depend fully upon $\hat{H}_m^{(1)}$. \square

Thus with j stagnating iterations at the end of the first cycle, the first j columns of $\hat{H}_m^{(2)}$ cannot be prescribed anyhow. For the first row of these columns we know the following.

LEMMA 2.5. *If the residual norms in the initial cycle satisfy*

$$\|r_0^{(1)}\| \geq \|r_1^{(1)}\| \geq \dots \geq \|r_{m-j-1}^{(1)}\| > \|r_{m-j}^{(1)}\| = \dots = \|r_m^{(1)}\|$$

for a nonnegative integer j smaller than or equal to m , then the first row of $\hat{H}_{1,j}^{(2)}$ is zero.

Proof. By Lemma 2.2 we have

$$\hat{H}_m^{(2)} = Z_{m+1}^* H Z_m, \quad Z_{m+1}e_1 = \begin{bmatrix} \gamma^{(1)} \\ 0 \end{bmatrix}, \quad (2.10)$$

where, as explained in the proof of Lemma 2.4, the vector $Z_m e_1$ is zero from position $m+2-j$ on and every new column of Z_m will have a new position with nonzero entry. The first Arnoldi vector having a nonzero entry on position $m+1$ is $Z_m e_{j+1}$. Using (2.10), this gives for the first row of $\hat{H}_{1,j}^{(2)}$

$$e_1^T \begin{bmatrix} \hat{H}_m^{(2)} \\ 0 \end{bmatrix} e_i = \begin{bmatrix} \gamma^{(1)*} & 0 \end{bmatrix} H Z_m e_i = \gamma^{(1)*} \hat{H}_m^{(1)} \begin{bmatrix} e_1^T Z_m e_i \\ \vdots \\ e_{m-j+i}^T Z_m e_i \\ 0 \\ \vdots \end{bmatrix}, \quad i = 1, \dots, j.$$

All these entries on the first row are zero because $\gamma^{(1)*} \hat{H}_m^{(1)}$ is the zero vector, see (2.4). \square

It is not difficult to see that the lemmas of this section can be formulated for any two subsequent restart cycles. Let us denote the residual vectors generated in the k th cycle of GMRES(m), $2 \leq k \leq N$, with $r_0^{(k)} = r_m^{(k-1)}, r_1^{(k)}, \dots, r_m^{(k)}$, and let us denote the Arnoldi decomposition generated during this cycle by

$$A V_m^{(k)} = V_{m+1}^{(k)} \hat{H}_m^{(k)}, \quad \text{where} \quad V_{m+1}^{(k)*} V_{m+1}^{(k)} = I_{m+1}, \quad V_{m+1}^{(k)} e_1 = V_{m+1}^{(k-1)} \gamma^{(k-1)}. \quad (2.11)$$

If $\hat{H}_m^{(k-1)}$ is decomposed as

$$\hat{H}_m^{(k-1)} = \begin{bmatrix} \chi_0^{(k-1)} & \dots & \chi_m^{(k-1)} \\ 0 & \Sigma_m^{(k-1)} & \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ I_m \end{bmatrix} \begin{bmatrix} \chi_0^{(k-1)} & \dots & \chi_{m-1}^{(k-1)} \\ 0 & \Sigma_{m-1}^{(k-1)} \end{bmatrix},$$

with $\chi_0^{(k-1)} = 1/\|r_0^{(k-1)}\|$ and $|\chi_i^{(k-1)}| = \left(1/\|r_i^{(k-1)}\|^2 - 1/\|r_{i-1}^{(k-1)}\|^2\right)^{\frac{1}{2}}$ for $i = 1, \dots, m$, (see Corollary 1.4), then the vector $\gamma^{(k-1)}$ is given by

$$\gamma^{(k-1)} = \|r_m^{(k-1)}\| \begin{bmatrix} \overline{\chi_0^{(k-1)}} \\ \vdots \\ \overline{\chi_m^{(k-1)}} \end{bmatrix}. \quad (2.12)$$

The proof is analogous to the proof of Lemma 2.2. The other lemmas of this section are formulated for any two subsequent restart cycles in the same way and the proofs are as for the first two cycles. Lemma 2.5 for arbitrary subsequent restart cycles leads to the following result.

THEOREM 2.6. *If the residual norms in the $(k-1)$ st cycle of GMRES(m), $mk < n$, satisfy*

$$\|r_0^{(k-1)}\| \geq \|r_1^{(k-1)}\| \geq \dots \geq \|r_{m-j-1}^{(k-1)}\| > \|r_{m-j}^{(k-1)}\| = \dots = \|r_m^{(k-1)}\|$$

for a nonnegative integer j smaller than or equal to m , then the residual norms in the k th cycle of GMRES(m) satisfy

$$\|r_0^{(k)}\| = \|r_1^{(k)}\| = \dots = \|r_j^{(k)}\|.$$

Proof. From Lemma 2.5 we know that the first j entries of the first row of $\hat{H}_m^{(k)}$ are zero. If we decompose $\hat{H}_m^{(k)}$ in the form (1.8) by consecutively finding the columns of the upper triangular matrix (starting with first column $e_1/\|r_0^{(k)}\|$), we see that $[\chi_0^{(k)}, \dots, \chi_{m-1}^{(k)}]$ is zero on positions 2 till $j+1$. With Corollary 1.4 this gives the claim. \square

This is a fascinating restriction which the residual norms of one cycle put on the residual norms in the subsequent cycle. A phase of stagnation at the end of some cycle is literally mirrored, with the same length, at the beginning of the next cycle. Equivalently, if a zero Ritz value appears during the last j subsequent iterations of a cycle, it must reappear in the first j iterations of the cycle that follows. The authors are not aware of any reference to this property in the literature, though the discussion in [29, Section 4] suggests that after stagnation in a cycle, restarting will produce little new information to overcome slow convergence.

Summarizing, it is not possible to prescribe for GMRES(m) any non-increasing convergence curve. As soon as we prescribe stagnation at the end of some cycle, the beginning of the next cycle must stagnate too; otherwise, the convergence curve is inadmissible. The next section will show that this is the *only* type of inadmissible convergence curve for GMRES(m).

3. Generating prescribed Hessenberg matrices. We will now assume that the very last iteration of each cycle does not stagnate. For that case, we show how to construct matrices and right-hand sides such that GMRES(m) generates prescribed Hessenberg matrices (and, therefore, also residual norms) in all N cycles where $Nm < n$. To begin with, we again consider the first two cycles.

Based on Lemma 2.2, we wish to find H in (2.9) such that $\hat{H}_m^{(2)}$ has prescribed entries. This is an „inverse” Arnoldi decomposition problem, where an input matrix has to be found to create an Arnoldi decomposition with some given properties. The first m columns of H are fully determined by $\hat{H}_m^{(1)}$, see (2.2). Thus we must concentrate on the choice of the columns $m+1$ until $2m$. The probably easiest way to satisfy (2.9) with $\hat{H}_m^{(2)}$ given, is to assume that the matrix Z_{m+1}

with orthonormal columns has a simple form. Assume that Z_{m+1} has the „canonical” form

$$\tilde{Z}_{m+1} \equiv \begin{bmatrix} \gamma^{(1)} & 0 \\ 0 & I_m \\ 0 & 0 \end{bmatrix}. \quad (3.1)$$

We will find the columns $m + 1$ until $2m$ of a matrix H satisfying (2.9) with this specific choice and we will denote this particular H with \tilde{H} . Equating the first column of

$$\tilde{H}\tilde{Z}_m = \tilde{Z}_{m+1}\hat{H}_m^{(2)} \quad (3.2)$$

gives

$$\tilde{H}\tilde{Z}_m e_1 = \begin{bmatrix} \hat{H}_m^{(1)} \\ 0 \end{bmatrix} \begin{bmatrix} \gamma_1^{(1)} \\ \vdots \\ \gamma_m^{(1)} \end{bmatrix} + \gamma_{m+1}^{(1)} \begin{bmatrix} \tilde{h}_{1,m+1} \\ \vdots \\ \tilde{h}_{m+2,m+1} \\ 0 \\ \vdots \end{bmatrix} = h_{1,1}^{(2)} \begin{bmatrix} \gamma^{(1)} \\ 0 \\ \vdots \end{bmatrix} + h_{2,1}^{(2)} e_{m+2},$$

where $h_{i,j}^{(2)}$ are the entries of $\hat{H}_m^{(2)}$. Therefore, the $(m + 1)$ st column of \tilde{H} must satisfy

$$\begin{bmatrix} \tilde{h}_{1,m+1} \\ \vdots \\ \tilde{h}_{m+1,m+1} \end{bmatrix} = \frac{1}{\gamma_{m+1}^{(1)}} \left(h_{1,1}^{(2)} \gamma^{(1)} - \hat{H}_m^{(1)} \begin{bmatrix} \gamma_1^{(1)} \\ \vdots \\ \gamma_m^{(1)} \end{bmatrix} \right), \quad \tilde{h}_{m+2,m+1} = \frac{h_{2,1}^{(2)}}{\gamma_{m+1}^{(1)}}. \quad (3.3)$$

The relation for the second column in $\tilde{H}\tilde{Z}_m = \tilde{Z}_{m+1}\hat{H}_m^{(2)}$,

$$\tilde{H}\tilde{Z}_m e_2 = \tilde{H}e_{m+2} = \begin{bmatrix} \tilde{h}_{1,m+2} \\ \vdots \\ \tilde{h}_{m+3,m+2} \\ 0 \end{bmatrix} = h_{1,2}^{(2)} \begin{bmatrix} \gamma^{(1)} \\ 0 \\ \vdots \\ 0 \end{bmatrix} + h_{2,2}^{(2)} e_{m+2} + h_{3,2}^{(2)} e_{m+3},$$

gives the entries of the $(m + 2)$ nd column of \tilde{H} :

$$\begin{bmatrix} \tilde{h}_{1,m+2} \\ \vdots \\ \tilde{h}_{m+1,m+2} \end{bmatrix} = h_{1,2}^{(2)} \gamma^{(1)}, \quad \tilde{h}_{m+2,m+2} = h_{2,2}^{(2)}, \quad \tilde{h}_{m+3,m+2} = h_{3,2}^{(2)}. \quad (3.4)$$

We can continue in this manner until the $2m$ th column of \tilde{H} , yielding, for $i = 3, \dots, m$,

$$\begin{bmatrix} \tilde{h}_{1,m+i} \\ \vdots \\ \tilde{h}_{m+1,m+i} \end{bmatrix} = h_{1,i}^{(2)} \gamma^{(1)}, \quad \tilde{h}_{m+\ell,m+i} = h_{\ell,i}^{(2)}, \quad \ell = 2, \dots, i + 1. \quad (3.5)$$

This choice of the first $2m$ columns of \tilde{H} guarantees that we generate the prescribed upper Hessenberg matrices $\hat{H}_m^{(1)}$ and $\hat{H}_m^{(2)}$.

We summarize the above discussion in a theorem and show that it can be extended to more than two cycles. In the statement of the next theorem we use that a non-singular $m \times m$ leading

principal submatrix of the generated Hessenberg matrix guarantees that there is no stagnation at the end of the corresponding GMRES(m) cycle (see, e.g., [3]).

THEOREM 3.1. *Let $A \in \mathbb{C}^{n \times n}$ be a matrix, $b \in \mathbb{C}^n$ be a nonzero vector and let for $Nm < n$,*

$$\hat{H}_m^{(1)}, \dots, \hat{H}_m^{(N)} \in \mathbb{C}^{(m+1) \times m}$$

be N unreduced upper Hessenberg matrices with real positive subdiagonal and with nonsingular leading $m \times m$ principal submatrix. Then for all $k \leq N$, the k th cycle of GMRES(m) applied to A and b generates the Hessenberg matrix $\hat{H}_m^{(k)}$ if the matrix A and the vector b have the following form:

$$A = V\tilde{H}V^*, \quad b = \|b\|Ve_1, \quad (3.6)$$

where V is unitary, \tilde{H} is upper Hessenberg, the $(m+1) \times m$ upper left submatrix of \tilde{H} equals $\hat{H}_m^{(1)}$ and for all k , $2 \leq k \leq N$, the columns $(k-1)m+1$ till km of \tilde{H} (i.e., those corresponding to the k th cycle) begin with a transition column

$$\tilde{H}e_{(k-1)m+1} = \Gamma^{(1)} \dots \Gamma^{(k-2)} \begin{bmatrix} t^{(k-1)} \\ 0 \\ \vdots \end{bmatrix}, \quad (3.7)$$

(the product $\Gamma^{(1)}\Gamma^{(0)}$ being defined as I_n) and the remaining columns are of the form

$$\tilde{H}[e_{(k-1)m+2}, \dots, e_{km}] = \Gamma^{(1)} \dots \Gamma^{(k-1)} \begin{bmatrix} \hat{H}_m^{(k)} \begin{bmatrix} 0 \\ I_{m-1} \end{bmatrix} \\ \vdots \end{bmatrix}. \quad (3.8)$$

Here $t^{(k)} = [t_1^{(k)}, \dots, t_{m+2}^{(k)}]^T$ with

$$\begin{bmatrix} t_1^{(k)} \\ \vdots \\ t_{m+1}^{(k)} \end{bmatrix} = \frac{1}{\gamma_{m+1}^{(k)}} \left(h_{1,1}^{(k+1)} \gamma^{(k)} - \hat{H}_m^{(k)} \begin{bmatrix} \gamma_1^{(k)} \\ \vdots \\ \gamma_m^{(k)} \end{bmatrix} \right), \quad t_{m+2}^{(k)} = \frac{h_{2,1}^{(k+1)}}{\gamma_{m+1}^{(k)}} \quad (3.9)$$

where $\gamma^{(k)}$ is as defined in (2.12) and

$$\Gamma^{(k)} = \begin{bmatrix} \gamma^{(k)} & 0 & 0 \\ 0 & I_{n-m-1} & 0 \end{bmatrix} \in \mathbb{C}^{n \times n}, \quad k = 1, \dots, N-1. \quad (3.10)$$

Proof. A and b generate $\hat{H}_m^{(1)}$ in the initial cycle because the $(m+1) \times m$ upper left submatrix of \tilde{H} equals $\hat{H}_m^{(1)}$. For $k = 2$, the transition column (3.9) corresponds to (3.3), the column $m+2$,

$$\tilde{H}e_{m+2} = \Gamma^{(1)} \begin{bmatrix} \hat{H}_m^{(2)} e_2 \\ 0 \\ \vdots \end{bmatrix},$$

to (3.4) and the remaining columns in (3.8) to (3.5). For $k = 3$, we realize that $\hat{H}_m^{(3)}$ is generated if

$$\tilde{H}\tilde{Z}_{2m} = \tilde{Z}_{2m+1} \begin{bmatrix} \hat{H}_m^{(2)} & & & \\ & t^{(2)} & & \\ & & \Gamma^{(2)} & \\ & 0 & & \hat{H}_m^{(3)} \begin{bmatrix} 0 \\ I_{m-1} \\ 0 \\ \vdots \end{bmatrix} \end{bmatrix},$$

where we use the results proved for $k = 2$. By equating column $m + 1$ in this equation we obtain the transition column

$$\tilde{H}e_{2m+1} = \Gamma^{(1)} \begin{bmatrix} t^{(2)} \\ 0 \\ \vdots \end{bmatrix}$$

and by equating columns $m + 2$ till $2m$ we obtain

$$\tilde{H}[e_{2m+2}, \dots, e_{3m}] = \Gamma^{(1)}\Gamma^{(2)} \begin{bmatrix} \hat{H}_m^{(3)} \begin{bmatrix} 0 \\ I_{m-1} \\ 0 \\ \vdots \end{bmatrix} \end{bmatrix}.$$

The cases $k > 3$ are obtained in the same way. \square

An illustration of the previous theorem is given in the example in Section 4. The theorem shows how to prescribe *all* the Hessenberg matrices generated during all the iterations of N restarts as long as $Nm < n$ and as long as no cycle stagnates in its last iteration. By the choice of the entries of these Hessenberg matrices, we can prescribe the GMRES(m) residual norms during N restart cycles, see Corollary 1.4. The same corollary shows how to additionally force the Ritz values of the cycles to take prescribed values. We remark that other choices of the entries of the Hessenberg matrices might prescribe other interesting values. For example, in [9, Section 6.3] it is shown that the singular values can be prescribed. As for the spectrum of the system matrix, we can use the following.

LEMMA 3.2. *Let H be an unreduced upper Hessenberg matrix of size n whose leading $n - 1$ columns are given and consider n complex numbers $\lambda_1, \dots, \lambda_n$. The last column of H can be chosen such that H has the eigenvalues $\lambda_1, \dots, \lambda_n$.*

Proof. See [7, Theorem 2.2] or [25, Theorem 3]. \square

Due to the fact that $Nm < n$, Theorem 3.1 does not put any conditions on the last column of \tilde{H} and it can always be chosen such that \tilde{H} (and hence A) has a prescribed spectrum.

It is possible to formulate Theorem 3.1 where the case of stagnation at the end of cycles is incorporated. But the resulting Hessenberg matrix \tilde{H} in the parametrization $A = V\tilde{H}V^*$ is more difficult to describe. The main complication is that when we prescribe stagnation during the last j iterations of some cycle, this fully determines the first j columns of the Hessenberg matrix for the next cycle, see Lemma 2.4. To give the remaining columns some prescribed entries, it suffices to properly define only $m - j + 1$ new columns of the Hessenberg matrix \tilde{H} , instead of m new columns. Therefore the number of columns needed to prescribe $\hat{H}_m^{(k)}$ will depend on the length of stagnation at the end of the $(k - 1)$ st cycle. This also means that when we allow stagnation at the end of cycles, we can prescribe non-increasing residual norms during *more* than n iterations of GMRES(m) while having conditions for *less* than Nm , $Nm < n$ columns of \tilde{H} . Again, as we

have no conditions for the entries of the last column of \tilde{H} , we can exploit Lemma 3.2 to prescribe the spectrum of $A = V\tilde{H}V^*$.

We can summarize the main results proved for the possible behavior of restarted GMRES.

PROPOSITION 3.3. *Let n, m be positive integers such that $m < n$. GMRES(m) can generate, for a linear system of size n with a matrix having any spectrum, any non-increasing convergence curve of the form*

$$\begin{aligned} \|r_0^{(1)}\| &\geq \|r_1^{(1)}\| \geq \cdots \geq \|r_{m-j_1-1}^{(1)}\| > \|r_{m-j_1}^{(1)}\| = \cdots = \|r_m^{(1)}\| = \\ \|r_0^{(2)}\| &= \|r_1^{(2)}\| = \cdots = \|r_{j_1}^{(2)}\| \geq \cdots \geq \|r_{m-j_2-1}^{(2)}\| > \|r_{m-j_2}^{(2)}\| = \cdots = \|r_m^{(2)}\| = \\ &\vdots \\ \|r_0^{(N)}\| &= \|r_1^{(N)}\| = \cdots = \|r_{j_{N-1}}^{(N)}\| \geq \cdots \geq \|r_{m-j_N-1}^{(N)}\| > \|r_{m-j_N}^{(N)}\| = \cdots = \|r_m^{(N)}\|, \end{aligned}$$

where the total number of cycles N is such that $\sum_{k=1}^N (m - j_k) < n$. The Ritz values generated in the initial cycle and in iterations corresponding to the residual norms

$$\|r_{j_{k-1}+1}^{(k)}\| \geq \cdots \geq \|r_m^{(k)}\|, \quad k = 2, \dots, N$$

can be any complex values as long as there is a zero Ritz value in every stagnating iteration.

4. Relation with full GMRES. We start this section with an investigation of the relation between our construction to prescribe the behavior of GMRES(m) and full GMRES. It turns out that full GMRES applied to the linear systems constructed in Section 3 can be carried out with short recurrences.

THEOREM 4.1. *Consider the linear system (3.6) in Theorem 3.1. The residual norms generated when GMRES(m) is applied to this system are the same as when full GMRES is applied to this system.*

Proof. The first m residual norms are trivially identical. For the rest of the proof we will compare the sizes of the values χ_i from Lemma 1.3; if they are equal, the residual norms are equal as well. The first χ_i for the first restart are, with Lemma 1.3,

$$\chi_0^{(2)} \equiv \frac{1}{\|r_0^{(2)}\|}, \quad \chi_1^{(2)} \equiv \frac{-\chi_0^{(2)} h_{1,1}^{(2)}}{h_{2,1}^{(2)}}. \quad (4.1)$$

The value χ_{m+1} for full GMRES is

$$\chi_{m+1} = \frac{-1}{\tilde{h}_{m+2,m+1}} [\chi_0, \dots, \chi_m]^T \begin{bmatrix} \tilde{h}_{1,m+1} \\ \vdots \\ \tilde{h}_{m+1,m+1} \end{bmatrix}, \quad (4.2)$$

where the entries $\tilde{h}_{1,m+1} \dots, \tilde{h}_{m+1,m+1}$ are given by

$$\begin{bmatrix} \tilde{h}_{1,m+1} \\ \vdots \\ \tilde{h}_{m+1,m+1} \end{bmatrix} = \frac{1}{\gamma_{m+1}^{(1)}} \left(h_{1,1}^{(2)} \gamma^{(1)} - \hat{H}_m^{(1)} \begin{bmatrix} \gamma_1^{(1)} \\ \vdots \\ \gamma_m^{(1)} \end{bmatrix} \right), \quad \tilde{h}_{m+2,m+1} = \frac{h_{2,1}^{(2)}}{\gamma_{m+1}^{(1)}}, \quad (4.3)$$

see (3.7) and (3.3). If we multiply the first equality in (4.3) with $[\chi_0, \dots, \chi_m]^T$ we have for its first term $[\chi_0, \dots, \chi_m]^T h_{1,1}^{(2)} \gamma^{(1)} = \chi_0^{(2)} h_{1,1}^{(2)}$ because $[\chi_0, \dots, \chi_m]^T \gamma^{(1)} = 1/\|r_m^{(1)}\| = \chi_0^{(2)}$, see Lemma 1.3. The second term is zero because of (2.4). Substituting in (4.2) gives $\chi_{m+1} = \frac{-\chi_0^{(2)} h_{1,1}^{(2)}}{h_{2,1}^{(2)}}$, which equals the second expression in (4.1).

The second value χ_i after the first restart is, with Lemma 1.3,

$$\chi_2^{(2)} \equiv \frac{-[\chi_0^{(2)}, \chi_1^{(2)}]^T \begin{bmatrix} h_{1,2}^{(2)} \\ h_{2,2}^{(2)} \end{bmatrix}}{h_{3,2}^{(2)}}.$$

For full GMRES we have

$$\chi_{m+2} = \frac{-[\chi_0, \dots, \chi_m]^T \gamma^{(1)} h_{1,2}^{(2)} - \chi_{m+1} h_{2,2}^{(2)}}{h_{3,2}^{(2)}},$$

see (3.4). Thus $\chi_{m+2} = \chi_2^{(2)}$. The equality of all other χ_i , and therefore of all other residual norms follows by induction. \square

Thus the linear systems we had constructed in Theorem 3.1 to generate prescribed GMRES(m) residual norms represent in fact the best case scenario for restarted GMRES: It converges as fast as full GMRES. In other words, the GMRES minimization process (1.2) can for these systems be carried out with $m+1$ -term recurrences. As will become clear later in this section, this surprising property is due to the special choice (3.1) used to construct the linear systems. The choice implies that nearly all Arnoldi vectors generated in full GMRES are orthogonal to the Arnoldi vectors in the restart cycles (this is in fact the situation where $\kappa(\mathcal{V}_{2m+1}) = 1$ in [29, Corollary 6.3]). By the Faber-Manteuffel theorem, the fact that the orthogonal bases for the Krylov subspaces associated with the linear systems in Theorem 3.1 can be computed with $m+1$ -term recurrences means that the involved matrices are normal of degree $m-1$, see, e.g. [15],[22, Chapter 4],[14].

An interesting consequence of the optimality property for GMRES(m) applied to the systems constructed in Theorem 3.1 is that no other restart length than m can give faster convergence (as no restart length converges faster than full GMRES). In particular, not even *larger* restart lengths produce convergence faster than GMRES(m) for the systems constructed in Theorem 3.1. Thus we have found a class of systems exhibiting the very counterintuitive behavior encountered sometimes in practice, where a larger restart parameter slows down convergence speed (see also [12], [10]).

We give an example for illustration. Suppose we wish to construct a linear system $Ax = b$ with $A \in \mathbb{R}^{16 \times 16}$, $b \in \mathbb{R}^{16}$, such that the residual norm history for GMRES(5) is

$$\begin{aligned} \left[\|r_0^{(1)}\|, \|r_1^{(1)}\|, \dots, \|r_5^{(1)}\| \right] &= [1, 0.7, 0.4, 0.1, 0.07, 0.04], \\ \left[\|r_0^{(2)}\|, \|r_1^{(2)}\|, \dots, \|r_5^{(2)}\| \right] &= [0.04, 0.01, 0.007, 0.004, 0.001, 7 \cdot 10^{-4}], \\ \left[\|r_0^{(3)}\|, \|r_1^{(3)}\|, \dots, \|r_5^{(3)}\| \right] &= [7 \cdot 10^{-4}, 4 \cdot 10^{-4}, 10^{-4}, 7 \cdot 10^{-5}, 4 \cdot 10^{-5}, 10^{-5}]. \end{aligned} \quad (4.4)$$

The residual norms for the three restart cycles can be obtained by defining three appropriate Hessenberg matrices of size 6×5 using Corollary 1.4. In the product (1.8) the values χ_i are determined by the prescribed residual norms except for the phase angles. We will choose all these values to be positive and we will choose all three matrices Σ_5 in (1.8) to be the upper triangular matrix of ones (we are not interested in forcing specific Ritz values here). The resulting Hessenberg matrices $\hat{H}_5^{(1)}, \hat{H}_5^{(2)}, \hat{H}_5^{(3)}$ will be generated by GMRES(5) if we use the construction

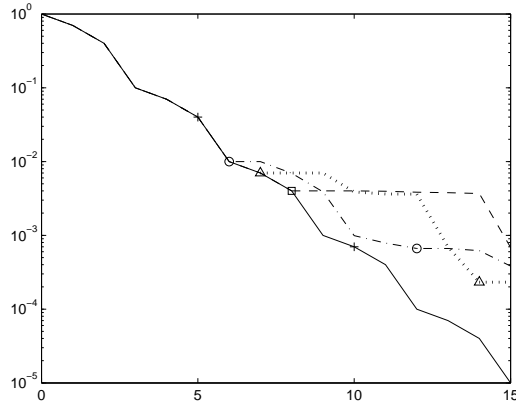


FIG. 4.1. GMRES residual norm curves for GMRES(5) (solid, crosses indicate restart), GMRES(6) (dash-dotted, circles indicate restart), GMRES(7) (dotted, triangles indicate restart) and GMRES(8) (dashed, squares indicate restart).

of Theorem 3.1. In our example we use $V \equiv I_{16}$ (though any other unitary V would give the same behavior reported below).

GMRES(5) applied to the linear systems constructed in this way produces the solid convergence curve in Figure 4.1. Of course, it corresponds with the residual norm history given in (4.4). Our experiment also confirms that full GMRES applied to the system yields the same solid curve. The other curves represent residual norms generated with larger restart lengths (6, 7 and 8). As explained, they do not reflect better convergence behavior than GMRES(5).

So far, we have constructed linear systems of the form (1.3) by finding conditions for the columns of H , based on the assumption that Z_{m+1} in (2.9) has the „canonical” form (3.1). Clearly, other forms may be possible and give additional ways to prescribe the Hessenberg matrices of the individual cycles. But they may lead to different (faster) convergence of full GMRES and of restarted GMRES with other restart lengths. Alternative ways to prescribe the first two Hessenberg matrices are given below.

LEMMA 4.2. *Let GMRES(m) be applied to a system of the form (1.3) where H is an unreduced upper Hessenberg matrix with real positive subdiagonal and let $\hat{H}_m^{(1)} \in \mathbb{C}^{(m+1) \times m}$ and $\hat{H}_m^{(2)} \in \mathbb{C}^{(m+1) \times m}$ be given unreduced upper Hessenberg matrices with real positive subdiagonal and nonsingular leading $m \times m$ principal submatrix. The first two restart cycles generate, subsequently, $\hat{H}_m^{(1)} \in \mathbb{C}^{(m+1) \times m}$ and $\hat{H}_m^{(2)} \in \mathbb{C}^{(m+1) \times m}$ if and only if the left upper block $\hat{H}_{2m} \in \mathbb{C}^{(2m+1) \times 2m}$ of H is of the form*

$$\hat{H}_{2m} = \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_m \\ 0 & R_m \end{bmatrix}^{-1} \tilde{H}_{2m} \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_{m-1} \\ 0 & R_{m-1} \end{bmatrix}, \quad (4.5)$$

where $\tilde{H}_{2m} \in \mathbb{C}^{(2m+1) \times 2m}$ is the left upper block of the Hessenberg matrix \tilde{H} defined in Theorem 3.1, $R_m \in \mathbb{C}^{m \times m}$ is a nonsingular upper triangular matrix with leading principal submatrix $R_{m-1} \in \mathbb{C}^{(m-1) \times (m-1)}$ such that $R_m^* R_m - I_m$ is positive semidefinite and $S_m \in \mathbb{C}^{m \times m}$ is a square matrix with first $m-1$ columns denoted by $S_{m-1} \in \mathbb{C}^{m \times (m-1)}$ such that

$$(\hat{H}_m^{(1)} S_m)^* \hat{H}_m^{(1)} S_m = R_m^* R_m - I_m. \quad (4.6)$$

Proof. Any unreduced upper Hessenberg matrix $\hat{H}_{2m} \in \mathbb{C}^{(2m+1) \times 2m}$ can be transformed into \tilde{H}_{2m} with a nonsingular upper triangular matrix. To see this, let us decompose \tilde{H}_{2m} and \hat{H}_{2m} as

$$\tilde{H}_{2m} = \tilde{U}_{2m+1} C_0 \tilde{U}_{2m}^{-1}, \quad \hat{H}_{2m} = U_{2m+1} C_0 U_{2m}^{-1}, \quad C_0 = \begin{bmatrix} 0 \\ I_{2m} \end{bmatrix} \quad (4.7)$$

(with \tilde{U}_{2m} resp. U_{2m} being the leading principal submatrix of size $2m$ of \tilde{U}_{2m+1} resp. U_{2m+1}) by equating consecutively the columns 1 till $2m$ of the equations $\tilde{H}_{2m} U_{2m} = U_{2m+1} C_0$ and $\hat{H}_{2m} \tilde{U}_{2m} = \tilde{U}_{2m+1} C_0$ with $U_{2m} e_1 = \tilde{U}_{2m} e_1 = e_1$. Then

$$\hat{H}_{2m} = X_{2m+1}^{-1} \tilde{H}_{2m} X_{2m}, \quad X_{2m+1} = \tilde{U}_{2m+1} U_{2m+1}^{-1}, \quad X_{2m} = \tilde{U}_{2m} U_{2m}^{-1}. \quad (4.8)$$

GMRES(m) applied to the system (1.3) generates in the initial cycle the Hessenberg matrix $\hat{H}_m^{(1)}$ if and only if

$$\begin{bmatrix} I_{m+1} & 0 \end{bmatrix} \hat{H}_{2m} \begin{bmatrix} I_m \\ 0 \end{bmatrix} = \hat{H}_m^{(1)} \Leftrightarrow \begin{bmatrix} I_{m+1} & 0 \end{bmatrix} X_{2m+1} \tilde{H}_{2m} X_{2m}^{-1} \begin{bmatrix} I_m \\ 0 \end{bmatrix} = \hat{H}_m^{(1)}.$$

Using the facts that the leading $(m+1) \times m$ submatrix of \tilde{H}_{2m} is equal to $\hat{H}_m^{(1)}$ and that X_{2m+1} is upper triangular, we obtain the equivalent condition that the leading principal submatrix of X_{2m+1} of size $m+1$ must be the identity matrix.

GMRES(m) applied to the system (1.3) generates in the second cycle the Hessenberg matrix $\hat{H}_m^{(2)}$ if and only if $H Z_m = Z_{m+1} \hat{H}_m^{(2)}$ with the columns of Z_{m+1} orthogonal to each other and $Z e_{m+1} = \begin{bmatrix} (\gamma^{(1)})^T & 0 \end{bmatrix}^T$ see Lemma 2.2. As this Arnoldi decomposition lives only on the left upper $(2m+1) \times 2m$ block it can also be written, with a slight abuse of notation, as $\tilde{H}_{2m} Z_m = Z_{m+1} \hat{H}_m^{(2)}$. Similarly, $\tilde{H}_{2m} \tilde{Z}_m = \tilde{Z}_{m+1} \hat{H}_m^{(2)}$, where \tilde{H} is defined in Theorem 3.1 (with $N = 2$) and

$$\tilde{Z}_{m+1} = \begin{bmatrix} \gamma^{(1)} & 0 \\ 0 & I_m \end{bmatrix} \in \mathbb{C}^{(2m+1) \times (m+1)}.$$

Thus $X_{2m+1} \hat{H}_{2m} X_{2m}^{-1} \tilde{Z}_m = \tilde{Z}_{m+1} \hat{H}_m^{(2)}$, see (4.8), and by comparison with $\hat{H}_{2m} Z_m = Z_{m+1} \hat{H}_m^{(2)}$ we have $Z_{m+1} = X_{2m+1}^{-1} \tilde{Z}_{m+1}$. The matrix X_{2m+1} has the form

$$X_{2m+1} = \begin{bmatrix} I_{m+1} & Y \\ 0 & R_m \end{bmatrix}$$

and since the columns of Z_{m+1} must be orthonormal, we have

$$\begin{aligned} Z_{m+1}^* Z_{m+1} &= \tilde{Z}_{m+1}^* X_{2m+1}^{-*} X_{2m+1}^{-1} \tilde{Z}_{m+1} \\ &= \begin{bmatrix} \gamma^{(1)} & 0 \\ 0 & I_m \end{bmatrix}^* \begin{bmatrix} I_{m+1} & -Y R_m^{-1} \\ 0 & R_m^{-1} \end{bmatrix}^* \begin{bmatrix} I_{m+1} & -Y R_m^{-1} \\ 0 & R_m^{-1} \end{bmatrix} \begin{bmatrix} \gamma^{(1)} & 0 \\ 0 & I_m \end{bmatrix} \\ &= \begin{bmatrix} 1 & -(\gamma^{(1)})^* Y R_m^{-1} \\ -R_m^{-*} Y^* \gamma^{(1)} & (Y R_m^{-1})^* Y R_m^{-1} + R_m^{-*} R_m^{-1} \end{bmatrix} = I_{m+1}, \end{aligned}$$

where we used $\|\gamma^{(1)}\| = 1$. The orthogonal complement of $\gamma^{(1)}$ is the space generated by the columns of $\hat{H}_m^{(1)}$, see (2.4). Therefore the off-diagonal blocks are zero if and only if Y is of the form $\hat{H}_m^{(1)} S_m$. Then the trailing principal submatrix equals I_m if and only if (4.6) is satisfied. \square

Lemma 4.2 can be generalized for more than two cycles, thus giving alternatives to Theorem 3.1 for constructing linear systems with prescribed GMRES(m) residual norms (and prescribed Ritz values). In combination with Theorem 3.1, we then have a parametrization of the

entire class of linear systems yielding prescribed Hessenberg matrices for the first N cycles when $\text{GMRES}(m)$ is applied. The freedom allowed by the parametrization is in the choice of the unitary matrix V , in the individual upper triangular matrices R_m in (4.5) and of course in possibly undefined columns of H corresponding to cycles after the N th cycle (which can be used to prescribe the spectrum).

We may, by the choice of R_m , modify the residual norms for full GMRES while leaving the convergence of $\text{GMRES}(m)$ unchanged. Consider an $n \times n$ Hessenberg matrix H with left upper block $\tilde{H}_{2m} \in \mathbb{C}^{(2m+1) \times 2m}$ of the form (4.5), where \tilde{H}_{2m} is the left upper block of the matrix constructed from given matrices $\hat{H}_m^{(1)}$ and $\hat{H}_m^{(2)}$ according to Theorem 3.1. Then with Lemma 4.2, $\text{GMRES}(m)$ applied to any linear system of the form $A = HVV^*$, $b/\|b\| = Ve_1$ for a unitary V will generate subsequently $\hat{H}_m^{(1)}$ and $\hat{H}_m^{(2)}$ in the first two cycles.

Let us decompose \tilde{H}_{2m} and \hat{H}_{2m} in (4.5) as in (4.7). Because \tilde{H} is the matrix from Theorem 3.1, Theorem 4.1 tells us that it generates the same residual norms as $\text{GMRES}(m)$ when full GMRES is applied. Therefore, the first row of $(\tilde{U}_{2m})^{-1}$ contains entries χ_i satisfying

$$\chi_0 = \frac{1}{\|r_0^{(1)}\|}, \quad |\chi_i| = \sqrt{\frac{1}{\|r_i^{(1)}\|^2} - \frac{1}{\|r_{i-1}^{(1)}\|^2}}, \quad i = 1, \dots, m,$$

$$|\chi_{m+i}| = \sqrt{\frac{1}{\|r_i^{(2)}\|^2} - \frac{1}{\|r_{i-1}^{(2)}\|^2}}, \quad i = 1, \dots, m-1.$$

For the decomposition of the matrix \hat{H}_{2m} in (4.7), we have

$$U_{2m}^{-1} = (\tilde{U}_{2m})^{-1} \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_{m-1} \\ 0 & R_{m-1} \end{bmatrix}$$

and the first row $[\chi_0^F, \dots, \chi_{2m-1}^F]^T$ of U_{2m}^{-1} determines the residual norms generated when we apply full GMRES to H with right-hand side e_1 through

$$\chi_0^F = \frac{1}{\|r_0^F\|}, \quad |\chi_i^F| = \sqrt{\frac{1}{\|r_i^F\|^2} - \frac{1}{\|r_{i-1}^F\|^2}}, \quad i = 1, \dots, 2m-1.$$

For example, the $(m+2)$ nd entry of that row is

$$\chi_{m+1}^F = [\chi_0, \dots, \chi_{2m-1}] \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_{m-1} \\ 0 & R_{m-1} \end{bmatrix} e_{m+2} = \chi_{m+1} r_{1,1}, \quad (4.9)$$

where $r_{1,1}$ is the leading entry of R_m and where we used the property (2.4). As long as $\chi_{m+1} \neq 0$, the entry χ_{m+1}^F in (4.9) can be made equal to $\sqrt{\frac{1}{\|r_{m+1}^F\|^2} - \frac{1}{\|r_m^F\|^2}} \geq \chi_{m+1}$ with a number $r_{1,1}$ satisfying $|r_{1,1}| \geq 1$ (because $\|r_{m+1}^F\| \leq \|r_1^{(2)}\|$ always holds). Thus it may be possible to find an upper triangular matrix R_m with leading entry $r_{1,1}$ such that $R_m^* R_m - I_m$ is positive semidefinite. However, if in (4.9) $\chi_{m+1} = 0$, i.e. the first iteration of the restart cycle stagnates, then necessarily $\chi_{m+1}^F = 0$, i.e. full GMRES stagnates as well, regardless of the choice of R_m . Once more, the phenomenon of stagnation puts an interesting restriction on residual norms that can be prescribed. Clearly if we prescribe stagnation in iterations $m+1$ till $2m$ for full GMRES, then $\text{GMRES}(m)$ must stagnate, too. Surprisingly, the opposite is true as well provided there is no stagnation at the end of the first cycle. This fact is stated for general restart cycles in the following theorem.

THEOREM 4.3. *Let there be no stagnation at the end of the $(k-1)$ st restart cycle of $\text{GMRES}(m)$, $km < n$. If $\text{GMRES}(m)$ stagnates during the first j iterations of the k th cycle,*

then full GMRES applied to the same system stagnates as well in the corresponding iterations (i.e. in iterations $km + 1, \dots, km + j$).

Proof. We shall prove the claim for the initial and first restart cycle, the generalization for any two subsequent cycles being straightforward. It follows from Corollary 1.4 that if GMRES(m) stagnates during the first j iterations after its first restart, then the first row of $\hat{H}_m^{(2)}$ is zero on positions 1 till j . Let the linear system have the form (1.3). Because of Lemma 2.2 we have $\hat{H}_m^{(2)} = Z_{m+1}^* H Z_m$ with the first $m + 1$ entries of $Z_m e_1$ equal to $\gamma^{(1)}$; these entries are nonzero per assumption. Let h_{m+1} denote the $(m + 1)$ st column of H . Then

$$0 = e_1^T \hat{H}_m^{(2)} e_1 = [(\gamma^{(1)})^* \quad 0] \left(\hat{H}_m^{(1)} \begin{bmatrix} I_m & 0 \end{bmatrix} \gamma^{(1)} + h_{m+1} \gamma_{m+1}^{(1)} \right) = \gamma_{m+1}^{(1)} (\gamma^{(1)})^* h_{m+1},$$

where we used (2.4). Let \hat{h}_{m+1} denote the vector of the first $m + 1$ entries of h_{m+1} . Then $(\gamma^{(1)})^* h_{m+1} = 0$ implies $(\gamma^{(1)})^* \hat{h}_{m+1} = 0$. The orthogonal complement of $\gamma^{(1)}$ being spanned by the linearly independent columns of $\hat{H}_m^{(1)}$ ((2.4)), \hat{h}_{m+1} must be a linear combination of these columns. Hence the $(m + 1) \times (m + 1)$ leading principal submatrix of H is singular and full GMRES stagnates in the $(m + 1)$ st iteration. Using induction, the stagnation of the subsequent iterations follows analogously. \square

In other words, given a period of stagnation at the beginning of some cycle, the only way for full GMRES not to stagnate in corresponding iterations, is that GMRES(m) stagnated at the end of the previous cycle.

Leaving aside the effect of stagnation at the beginning of cycles, one may influence the residual norms of full GMRES by the choice of R_{m-1} in

$$\chi_{m+i}^F = [\chi_0, \dots, \chi_{2m-1}] \begin{bmatrix} I_{m+1} & \hat{H}_m^{(1)} S_{m-1} \\ 0 & R_{m-1} \end{bmatrix} e_{m+i+1}, \quad i = 1, \dots, m - 1.$$

With the values of χ_{m+i}^F given and using property (2.4), this amounts to finding an upper triangular matrix R_m such that

$$[\chi_{m+1}, \dots, \chi_{2m-1}] R_{m-1} = [\chi_{m+1}^F, \dots, \chi_{2m-1}^F]$$

and such that $R_m^* R_m - I_m$ is positive semidefinite. In the trivial case where $\chi_{m+i}^F = \chi_{m+i}$, $i = 1, \dots, m - 1$, R_m can be chosen as the identity matrix. But it is not difficult to see that other choices of R_m may result in $\chi_{m+i}^F = \chi_{m+i}$, $i = 1, \dots, m - 1$, as well. Thus the systems constructed in Theorem 3.1 appear not to be the unique systems where the full GMRES process can produce the same behavior as GMRES(m) and be computed with $m + 1$ -term recurrences (with prescribed upper Hessenberg matrices $\hat{H}_m^{(k)}$ for the individual cycles).

5. Conclusion. We showed that not any non-increasing convergence curve is possible for restarted GMRES. Stagnation at the end of a cycle is always repeated at the beginning of the next cycle. Thus it does not seem to be a good idea to restart GMRES with the current approximation if stagnation is observed. This is a strong motivation for restarting with other types of approximations. The previous section also showed that if restarted GMRES stagnates at the beginning of a cycle without stagnating at the end of the previous cycle, then even full GMRES stagnates in the corresponding iterations. Except for the phenomenon of propagated stagnation, all non-increasing convergence curves can be produced by GMRES(m) in the first n iterations and this is possible with any spectrum. It is also possible with any nonzero Ritz values generated in the individual cycles. Thus we proved an analogue of the result for full GMRES that residual norms can be independent from eigenvalues and Ritz values [7] and we described the form of the

class of matrices yielding prescribed residual norms, eigenvalues and Ritz values. Note that the presented parametrizations consider particular right-hand sides, but for a given b , matrices can always be constructed leading to the prescribed behavior (it suffices to have a unitary matrix V with first column equal to the scaled right-hand side b .) Our results might have consequences for other restarted Krylov subspace methods (like those used in restarted Arnoldi processes for eigenvalues (see, e.g., [2, 13]) and matrix function computations (see, e.g., [18])), though in our paper we considered only the specific restart with the current GMRES approximation.

As a by-product we found a class of linear systems for which full GMRES can be carried out with short, $m + 1$ -term recurrences. We explained that this class leads to the counterintuitive behavior of restarted GMRES where a larger restart length gives slower convergence. An interesting question is whether our results can be formulated for matrices with a given sparsity pattern, like those arising in finite differences or elements discretizations. We remark that the counterintuitive behavior of restarted GMRES just mentioned has been observed for sparse matrices resulting from standard five-point stencils [6]. We did not consider the situation where the Arnoldi orthogonalization process terminates early, but a technique to extend results to this situation was given in the end of [33]. We did not either address more iterations of GMRES(m) than the system size. This case, though not very relevant for practice, leads to an interesting theoretical challenge for possible future work.

Software. At the link http://www.cs.cas.cz/duintjertebbens/duintjertebbens_soft.html the reader can find MATLAB subroutines to create matrices and initial vectors with the parametrizations in this paper.

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