Any decreasing cycle–convergence curve is possible for restarted GMRES

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Abstract

Given a matrix order $n$, a restart parameter $m$ ($m < n$), a decreasing positive sequence $f(0) > f(1) > \ldots > f(q) > 0$, where $q < n/m$, it is shown that there exists an $n$-by-$n$ matrix $A$ and a vector $r_0$ with $\|r_0\| = f(0)$ such that $\|r_k\| = f(k)$, $k = 1, \ldots, q$, where $r_k$ is the residual at cycle $k$ of restarted GMRES with restart parameter $m$ applied to the linear system $Ax = b$, with initial residual $r_0 = b - Ax_0$. Moreover, the matrix $A$ can be chosen to have any desired eigenvalues. We can also construct arbitrary cases of stagnation; namely, when $f(0) > f(1) > \ldots > f(i) = f(i + 1) \geq 0$ for any $i < q$. The restart parameter can be fixed or variable.

1 Introduction

We consider the generalized minimal residual method (GMRES) [15] for solution of a nonsingular non-Hermitian systems of linear equations

$$Ax = b, \quad A \in \mathbb{C}^{n \times n}, \quad b \in \mathbb{C}^n. \quad (1)$$

For a few class of matrices, some convergence estimates are available for restarted GMRES and full GMRES. For example for real positive definite matrices (that is, for matrices $A$ for which $H = (A + A^H)/2$ is symmetric positive definite, or, equivalently, for matrices $A$ for which $x^H Ax > 0$ for any nonzero $x \in \mathbb{R}^n$), the Elman’s bound [6, 7, 11, 15] can be stated as follows

$$\|r_k\|^2 \leq (1 - \rho)^k \|r_0\|^2 \quad \text{where} \quad 0 < \rho \equiv (\lambda_{\min}(H)/\|A\|)^2 \leq 1.$$

The latter guarantees linear convergence of GMRES($m$) for any value of $m \geq 1$ for a positive definite matrix. Improvements and generalizations of this bound can be found in [3, 10, 21].

For normal matrices the convergence of both full and restarted GMRES is well studied. In particular, the convergence of full GMRES for normal matrices is known to be linear and there exist convergence estimates governed solely by the spectrum of $A$ [14, 18]. The convergence of restarted GMRES for normal matrices, however, is sublinear [2, 19]. The current paper is concerned with the general case.

For the general case, the following theorem proves that we can not prove convergence results based on the spectrum of the coefficient matrix alone.

Theorem 1 (Greenbaum, Pták, and Strakoš, 1996, [12]) Given a nonincreasing positive sequence $f(0) \geq f(1) \geq \ldots \geq f(n - 1) > 0$, there exists an $n$-by-$n$ matrix $A$ and a vector $r_0$ with $\|r_0\| = f(0)$ such that $f(k) = \|r_k\|$, $k = 1, \ldots, n - 1$, where $r_k$ is the residual at step $k$ of the GMRES algorithm applied to the linear system $Ax = b$, with initial residual $r_0 = b - Ax_0$. Moreover, the matrix $A$ can be chosen to have any desired eigenvalues.

This result states that, in general, eigenvalues alone do not determine the convergence of full GMRES. Assuming that the coefficient matrix $A$ is diagonalizable, some characterizations of the convergence of full GMRES rely on the condition number of the eigenbasis [18]. Other characterizations of the convergence of full GMRES rely on pseudospectra [14]. More commonly, the field of values is used [3, 6, 7, 11, 15, 16, 21]. A discussion on how descriptive some of these bounds are is given by Embree [8].

The main result of this paper is given in the abstract. We will repeat it here.
Theorem 2  Given a matrix order $n$, a restart parameter $m (m < n)$, a decreasing positive sequence $f(0) > f(1) > \ldots > f(q) \geq 0$, where $q < n/m$, there exits an $n$-by-$n$ matrix $A$ and a vector $r_0$ with $\|r_0\| = f(0)$ such that $\|r_k\| = f(k)$, $k = 1, \ldots, q$, where $r_k$ is the residual at cycle $k$ of restarted GMRES with restart parameter $m$ applied to the linear system $Ax = b$, with initial residual $r_0 = b - Ax_0$. Moreover, the matrix $A$ can be chosen to have any desired eigenvalues.

Section 2 contains a proof of Theorem 2. Theorem 2 is to restarted GMRES what Theorem 1 is to full GMRES. The proof we provide is constructive and directly inspired by the article of Greenbaum, Pták, and Strakoš [12]. Although Greenbaum, Pták, and Strakoš laid the path, there are several specific difficulties ahead in the case of restarted GMRES.

Full GMRES has a nonincreasing convergence (for any $i \geq 0$, $f(i) \geq f(i + 1)$) and it computes the exact solution in at most $n$ steps ($f(n) = 0$). It is remarkable that Greenbaum, Pták, and Strakoš are able to characterize any admissible convergence for GMRES. (See assumptions on $f$ in Theorem 1) At the same time we would like to note that the cycle-convergence of restarted GMRES can have two admissible scenarios: either for any $i$, $f(i) > f(i + 1)$, in other words, the cycle-convergence is decreasing; or there exists $s$ such that $f(i) > f(i + 1)$ for any $i < s$, and then for any $i > s$, $f(i) = f(s)$, in other words, if restarted GMRES stagnates at cycle $s + 1$, it stagnates forever. Then Theorem 2 considers the first case (decreasing cycle-convergence). In Section 3 we consider the second case (stagnation). Therefore with Theorem 2 and Section 3 we prove that any admissible cycle-convergence curve is possible for the $q$ first cycles of restarted GMRES.

As mentioned above, the maximum number of iterations of full GMRES is at most $n$, and the method delivers the exact solution in a finite number of steps. Restarted GMRES, however, may never provide the exact solution. It will (hopefully) decrease the residual norm at each cycle, that is, provide a more and more accurate approximation to the exact solution. With $n^2$ parameters in $A$ and $n$ parameters in $b$ we are not able to control the convergence for an infinite amount of cycles. For this reason, it is natural to consider only the first $q < n/m$ initial GMRES($m$) cycles. Actually, we provide the same level of control as Greenbaum, Pták, and Strakoš: $n$ iterations (or $q$ cycles with $q < n/m$) and $n$ eigenvalues.

In Section 4 we generalize the result given by Theorem 2 and Section 3 for the case of variable restart parameters. The sequence of restart parameters $m_k$ needs to be known a priori. We show that GMRES($m_k$) can produce any admissible cycle-convergence curve at the $q$ initial cycles, regardless of the spectrum of the coefficient matrix, where $q$ is such that $\sum_{i=1}^{q} m_k < n$. We note that our construction can be a reasonable tool for generating examples/counter-examples for different strategies for varying the restart parameter, e.g. [2].

The cycle-convergence of restarted GMRES for normal matrices is sublinear [2, 19]. However, for general matrices, through Theorem 2 one can expect any convergence curve. In particular, it is possible to construct matrices in which the convergence of GMRES($m$) is fast (e.g. superlinear). This relates to the observations of Zhong and Morgan [20] who report superlinear cycle-convergence for their particular cases of nonnormal matrices, as well as to [19], where it is shown that the cycle-convergence can become superlinear as the coefficient matrix departs from normality.

In a pedagogical paper, Embree [9] presents a 3-by-3 linear system of equations and attempts to solve it with GMRES(1) and GMRES(2). While GMRES(1) converges to the exact solution in 3 cycles, GMRES(2) (almost) stagnates. Our main result, basically, reaffirms this intuition in the sense that the increase in the restart parameter (and thus, in the computational complexity at each cycle) does not necessarily imply a faster convergence.

In order to improve the convergence of restarted GMRES, several techniques [11, 4, 5, 10, 13] have been proposed which consist of augmenting (or enriching) the Krylov space with eigenvectors or, alternatively, deflating some of the eigenvalues from the spectrum of the original matrix $A$. The eigenvalues targeted are the ones the closest from zero. These techniques have proved effective and the convergence of restarted GMRES is, in practice, greatly improved. Theorem 2 states that, in the general case, eigenvalues alone do not determine the convergence of restarted GMRES, therefore it is hard to provide a theoretical justification for the choice of removing the eigenvalues the closest from zero. A beginning of theoretical understanding has been provided by Zítko [22].

We have generated two Matlab functions that correspond to Theorem 1 and Theorem 2. Given a matrix size, a restart parameter, a convergence curve and a spectrum, we construct the appropriate matrix and right-hand side. See: http://www-math.cudenver.edu/~eugenev/edf.software/anycurve/.
The main message that we would like our readers to retain from this paper is that in the context of GMRES(m), for a certain number of initial cycles, any convergence curve is possible independently of the spectrum of the coefficient matrix. This means that eigenvalues alone do not determine the convergence of restarted GMRES.

2 Constructive proof of Theorem [2]

Let \( n \) be a matrix order and \( m \) a restart parameter \( (m < n) \), \( \Lambda = \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \subset \mathbb{C} \setminus \{0\} \) be a set of \( n \) nonzero complex numbers, and \( \{f(k)\}_{k=0}^{q} \) be a decreasing sequence of positive real numbers, \( q < n/m \).

In this section we construct a matrix \( A \in \mathbb{C}^{n \times n} \) and an initial residual vector \( r_0 = b - Ax_0 \in \mathbb{C}^n \) such that GMRES(m) applied to the system \( \mathbf{Ax} = \mathbf{b} \) with the initial approximate solution \( x_0 \), produces a sequence \( \{x_k\}_{k=1}^{q} \) of approximate solutions with corresponding residual vectors \( \{r_k\}_{k=0}^{q} \) having the prescribed norms: \( \|r_k\| = f(k) \). Moreover the spectrum of \( A \) is \( \Lambda \).

2.1 Outline of the proof

The general approach described in this paper is similar to the approach of Greenbaum, Ptáč, and Strakos [12]:

we fix an initial residual vector, construct an appropriate basis of \( \mathbb{C}^n \) and use this basis to define a linear operator \( A \). This operator is represented by the matrix \( A \) in the canonical basis. It has the prescribed spectrum and provides the desired cycle–convergence at the first \( q \) cycles of GMRES(m). However, the presence of restarts somewhat complicates the construction: the choice of the basis vectors, as well as the structure of the resulting operator \( A \), becomes less transparent. Below we describe our three-step construction.

At the first step we construct \( q \) sets of vectors \( W_m^{(k)} = \{w_1^{(k)}, \ldots, w_m^{(k)}\}, k = 1, \ldots, q \), each set \( W_m^{(k)} \) is the orthonormal basis of the Krylov residual subspace \( AK_m (A, r_{k-1}) \) generated at the \( k \)-th GMRES(m) cycle such that

\[
\text{span} \ W_j^{(k)} = AK_j (A, r_{k-1}), \quad j = 1, \ldots, m.
\] (2)

(With this definition, \( W_m^{(k)} \) is defined up to multiplication by a complex number of unit modulus.)

The orthonormal basis \( W_m^{(k)} \) needs to be chosen in order to generate residual vectors \( r_k \) with the prescribed norms \( f(k) \) at the end of each cycle subject to the additional requirement that the set of \( mq + 1 (\leq n) \) vectors

\[
\mathfrak{S} = \{r_0, w_1^{(1)}, \ldots, w_{m-1}^{(1)}, r_1, w_1^{(2)}, \ldots, w_{m-1}^{(2)}, \ldots, r_{q-1}, w_1^{(q)}, \ldots, w_{m-1}^{(q)} \}
\] (3)

is linearly independent.

Once we have the set \( \mathfrak{S} \), we will complete it to have a basis for \( \mathbb{C}^n \). When the number of vectors in \( \mathfrak{S} \) is less than \( n \), a basis \( S \) of \( \mathbb{C}^n \) is obtained by completion of \( \mathfrak{S} \) with a set \( S \) of \( n - mq - 1 \) vectors, i.e. \( S = \{\mathfrak{S}, \hat{S}\} \).

This will provide a representation of \( \mathbb{C}^n \) as the direct sum

\[
\mathbb{C}^n = \text{span} \ S = \text{span}\{r_0, W_m^{(1)}\} \oplus \cdots \oplus \text{span}\{r_{q-1}, W_m^{(q)}\} \oplus \text{span}\{r_q, \hat{S}\}.
\] (4)

The latter translates in terms of Krylov subspaces into

\[
\mathbb{C}^n = \text{span} \ S = K_m (A, r_0) \oplus \cdots \oplus K_m (A, r_{q-1}) \oplus \text{span}\{r_q, \hat{S}\}.
\]

At the second step of our construction, we define a linear operator \( A : \mathbb{C}^n \to \mathbb{C}^n \) with spectrum \( \Lambda \) which generates the Krylov residual subspaces in Eq. (2) at each GMRES(m) cycle, by its action on the basis vectors \( S \), such that the desired matrix \( A \) is the operator \( A \)'s representation in the canonical basis. The third step accomplishes the construction by a similarity transformation.

The two following subsections are concerned with the question if \( [2] \), \( [3] \), \( [4] \) and the definition of the operator \( A \) with the prescribed spectrum is actually possible.
2.2 Step 1: Construction of a sequence of Krylov subspaces which provide the prescribed cycle–convergence

At the \( k \)-th GMRES\((m) \) cycle, the residual vector \( r_k \) satisfies the following minimality condition:

\[
\|r_k\| = \min_{u \in AK_m(A, r_{k-1})} \|r_{k-1} - u\|. \tag{5}
\]

We assume that each set \( W^{(k)}_m \) is an orthonormal basis of a corresponding Krylov residual subspace \( AK_m(A, r_{k-1}) \), therefore the condition (5) implies

\[
r_k = r_{k-1} - \sum_{j=1}^{m} \langle r_{k-1}, w_j^{(k)} \rangle w_j^{(k)}, \quad k = 1, \ldots, q. \tag{6}
\]

At this stage, in order to simplify the forthcoming justification of the linear independence of the set \( S \), we impose a stricter requirement on the residual change inside the cycle. We will require that the residual vector \( r_{k-1} \) remains constant during the first \( m-1 \) inner steps of GMRES and is reduced only at the last, \( m \)-th, step. Thus, the equality in (6) can be written as

\[
r_k = r_{k-1} - \langle r_{k-1}, w_m^{(k)} \rangle w_m^{(k)}, \quad k = 1, \ldots, q. \tag{7}
\]

This implies that the vectors \( w_j^{(k)} \), \( j = 1, \ldots, m-1 \), are orthogonal to the residual vector \( r_{k-1} \), i.e.

\[
\langle r_{k-1}, w_j^{(k)} \rangle = 0, \quad j = 1, \ldots, m-1, \quad k = 1, \ldots, q. \tag{8}
\]

From Eq. (7), using the fact that \( r_k \perp w_m^{(k)} \) and the Pythagorean theorem, we obtain

\[
\|\langle r_{k-1}, w_m^{(k)} \rangle\| = \sqrt{\|r_{k-1}\|^2 - \|r_k\|^2}, \quad k = 1, \ldots, q.
\]

We rewrite the expression above in terms of cosines of angles \( \psi_k = \angle(r_{k-1}, w_m^{(k)}) \) by prescribing the expected values \( f(k) \) for the norms of the residuals. We get

\[
\cos \psi_k = \frac{\sqrt{f(k-1)^2 - f(k)^2}}{f(k-1)} \in (0, 1), \quad k = 1, \ldots, q. \tag{9}
\]

This latter equation means that, if we are given \( r_{k-1} \), one way to ensure the desired cycle–convergence at cycle \( k \) of GMRES\((m) \) is to choose the unit vectors \( w_j^{(k)} \) such that (7)–(9) holds.

In the following lemma, we show constructively that the described approach (7)–(9) leads to an appropriate set \( S \).

**Lemma 1** Given an initial vector \( r_0 \), \( \|r_0\| = f(0) \), there exist vectors \( r_k \), \( \|r_k\| = f(k) \) and orthonormal sets \( W^{(k)}_m \) such that Eq. (7), (8) and (9) hold, and the set \( S \) is linearly independent, \( k = 1, \ldots, q < n/m \).

**Proof.** The proof is by induction.

Let \( k = 1 \). Given the initial vector \( r_0 \), \( \|r_0\| = f(0) \), we pick \( W^{(1)}_{m-1} = \{w_1^{(1)}, \ldots, w_{m-1}^{(1)}\} \) an orthonormal set in \( r_0 \) in order to satisfy Eq. (5). The set \( \{r_0, W^{(1)}_{m-1}\} \) is linearly independent.

In order to choose the unit vector \( w_m^{(1)} \) orthogonal to the previously constructed vectors \( W^{(1)}_{m-1} \) and satisfying Eq. (9), we introduce a unit vector \( y^{(1)} \in \{r_0, W^{(1)}_{m-1}\}^\perp \), so that

\[
w_m^{(1)} = \frac{r_0}{f(0)} \cos \psi_1 + y^{(1)} \sin \psi_1.
\]

We find the vector \( r_1 \) by satisfying Eq. (7). Eq. (8) guarantees that \( \|r_1\| = f(1) \), as desired. Finally, we append the constructed vector \( r_1 \) to \( \{r_0, W^{(1)}_{m-1}\} \) and get the set \( \{r_0, W^{(1)}_{m-1}, r_1\} \), which is linearly independent, since, by construction, \( r_1 \) is not in span \( \{r_0, W^{(1)}_{m-1}\} \).
The induction assumption is that we have constructed \( k - 1 \) vectors \( r_1, \ldots, r_{k-1} \) with the prescribed norms \( f(1), \ldots, f(k-1) \) and orthonormal sets \( \mathcal{W}_m^{(1)}, \ldots, \mathcal{W}_m^{(k-1)} \), such that the equalities \( \mathcal{I} \), \( \mathcal{S} \) and \( \mathcal{M} \) hold, and the set
\[
\{ r_0, \mathcal{W}_m^{(1)} W_{m-1}^{(k-1)}, r_{k-1} \}
\]
is linearly independent. We want to show that we can construct the next vector \( r_k, \| r_k \| = f(k) \), and the orthonormal set \( \mathcal{W}_m^{(k)} \), satisfying Eq. \( \mathcal{I} \), \( \mathcal{S} \) and \( \mathcal{M} \), such that
\[
\{ r_0, \mathcal{W}_m^{(1)} W_{m-1}^{(k-1)}, r_{k-1}, \mathcal{W}_m^{(k)}(k), r_{k-1, m-1}, r_k \}
\]
is linearly independent, \( k \leq q \).

We start by constructing orthonormal vectors \( \mathcal{W}_m^{(k)}(k) = \{ w_1^{(k)}, \ldots, w_m^{(k)} \} \), satisfying Eq. \( \mathcal{S} \), with the additional requirement that the set \( \mathcal{W}_m^{(k)}(k) \) is not in the span of the previously constructed vectors given in the set \( \mathcal{M} \). From these considerations we choose \( \mathcal{W}_m^{(k)}(k) \) as an orthonormal set in the orthogonal complement of \( \mathcal{M} \), i.e.
\[
w_j^{(k)} \in \{ r_0, \mathcal{W}_m^{(1)} W_{m-1}^{(k-1)}, r_{k-1} \}, j = 1, \ldots, m - 1.
\]
Appending \( \mathcal{W}_m^{(k)}(k) \) to the set \( \mathcal{M} \) will give a linearly independent set.

To finish the proof, we need to construct the vector \( w_m^{(k)} \), satisfying Eq. \( \mathcal{I} \) and orthogonal to \( \mathcal{W}_m^{(k)}(k) \). For this reason we introduce a unit vector \( y^{(k)} \),
\[
y^{(k)} \in \{ r_0, \mathcal{W}_m^{(1)} W_{m-1}^{(k-1)}, r_{k-1}, \mathcal{W}_m^{(k)}(k) \},
\]
so that \( w_m^{(k)} \)
\[
w_m^{(k)} = \frac{r_{k-1}}{f(k-1)} \cos \psi_k + y^{(k)} \sin \psi_k.
\]

We define the vector \( r_k \) with Eq. \( \mathcal{I} \). Eq. \( \mathcal{I} \) guarantees \( \| r_k \| = f(k) \). The set \( \mathcal{M} \) is linearly independent, since, by construction, the vector \( r_k \) is not in span \( \{ r_0, \mathcal{W}_m^{(1)} W_{m-1}^{(k-1)}, r_{k-1} \} \).

\[\square\]

2.3 Step 2: Definition of a linear operator with any prescribed spectrum

So far we have shown that, given an initial residual vector \( r_0, \| r_0 \| = f(0) \), it is possible to construct vectors \( r_k, \| r_k \| = f(k) \), and orthonormal vectors \( \mathcal{W}_m^{(k)}(k), k = 1, \ldots, q \), satisfying Eq. \( \mathcal{I} \), \( \mathcal{S} \) and \( \mathcal{M} \), such that the set \( \mathcal{S} \) of \( mq + 1 \) vectors is linearly independent.

In order to define a unique linear operator, we need to have a valid basis of \( \mathbb{C}^n \) on hand. Thus, we expand the set \( \mathcal{S} \) by linearly independent vectors \( \mathcal{S} = \{ \hat{s}_1, \ldots, \hat{s}_t \}, t = n - mq - 1 \):
\[
\mathcal{S} = \{ r_0, \mathcal{W}_m^{(1)} W_{m-1}^{(q)}, r_q, \mathcal{W}_m^{(q)}, \hat{s}_1, \ldots, \hat{s}_t \},
\]
so that \( \mathcal{S} \) is a basis of \( \mathbb{C}^n \).

Before we define a linear operator \( \mathcal{A} \), let us consider the set \( \Lambda = \{ \lambda_1, \lambda_2, \ldots, \lambda_n \} \) of nonzero numbers in the complex plane that will define \( \mathcal{A} \)’s spectrum. We split \( \Lambda \) into \( q + 1 \) disjoint subsets
\[
\Lambda = \{ \Lambda_1, \Lambda_2, \ldots, \Lambda_q, \Lambda_{q+1} \},
\]
such that each \( \Lambda_k, k = 1, \ldots, q \), contains \( m \) elements of \( \Lambda \), and the remaining \( n - mq \) elements are included into \( \Lambda_{q+1} \).

For each set \( \Lambda_k \) we define a monic polynomial \( p_k(x) \), such that the roots of this polynomial are exactly the elements of the corresponding \( \Lambda_k \):
\[
p_k(x) = x^m - \sum_{j=0}^{m-1} \alpha_j^{(k)} x^j, \quad k = 1, \ldots, q; \tag{13}
\]
\[
p_{q+1}(x) = x^{t+1} - \sum_{j=0}^{t} \alpha_j^{(q+1)} x^j, \quad t = n - mq - 1; \tag{14}
\]
with $\alpha^{(k)}_{j}$’s being the coefficients of the respective polynomials, $\alpha^{(k)}_{0} \neq 0$, $k = 1, \ldots, q + 1$. $p_k(x)$ can be considered as the characteristic polynomial of an $m \times m$ matrix with spectrum $\Lambda_k$. $p_{q+1}(x)$ can be considered as the characteristic polynomial of a $(t + 1)$-by-$(t + 1)$ matrix with spectrum $\Lambda_{q+1}$.

We define the operator $A : \mathbb{C}^n \rightarrow \mathbb{C}^n$ as follow:

$$
\begin{align*}
A\bar{r}_{k-1} &= w^{(k)}_1, \\
A\bar{w}^{(k)}_1 &= w^{(k)}_2, \\
&\vdots \\
A\bar{w}^{(k)}_{m-2} &= w^{(k)}_{m-1}, \\
A\bar{w}^{(k)}_{m-1} &= -\alpha^{(k)}_0 \bar{r}_k + \alpha^{(k)}_0 \bar{r}_{k-1} + \alpha^{(k)}_1 \bar{w}^{(k)}_1 + \cdots + \alpha^{(k)}_{m-1} \bar{w}^{(k)}_{m-1}, \quad k = 1, \ldots, q; \\
A\bar{r}_q &= \bar{s}_1, \\
A\bar{s}_1 &= \bar{s}_2, \\
&\vdots \\
A\bar{s}_{t-1} &= \bar{s}_t, \\
A\bar{s}_t &= \alpha^{(q+1)}_0 \bar{r}_q + \alpha^{(q+1)}_1 \bar{s}_1 + \cdots + \alpha^{(q+1)}_t \bar{s}_t,
\end{align*}
$$

(15)

where $\alpha^{(k)}_{j}$’s are the coefficients of polynomials (13) and (14).

The following lemma shows that, given vectors $\bar{r}_k$ and orthonormal sets $\mathcal{W}^{(k)}_m$ constructed according to Lemma 1, the linear operator $A$, defined by (15) and represented by a matrix $A$ in the canonical basis, generates the desired Krylov residual subspaces given in Eq. (2); and the spectrum of $A$ can be arbitrarily chosen.

**Lemma 2** Let the initial residual vector $\bar{r}_0$, $\|\bar{r}_0\| = f(0)$, as well as the residual vectors $\bar{r}_k$ and orthonormal sets $\mathcal{W}^{(k)}_m$ be constructed according to Lemma 1. Let $S$ be the basis of $\mathbb{C}^n$ as defined by Eq. (12). We assume a matrix $A$ to be the representation in the canonical basis of the linear operator $A$ defined by Eq. (15). Then the linear operator $A$ generates the Krylov residual subspaces given in Eq. (2). Moreover, $A$ has the prescribed spectrum $\Lambda$.

**Proof.** Directly from the definition (15) of the linear operator $A$, for $k = 1, \ldots, q$, we have:

$$
\text{span}\{A\bar{r}_{k-1}, \ldots, A^{j}r_{k-1}\} = \text{span} \mathcal{W}^{(k)}_j, \quad j = 1, \ldots, m - 1.
$$

To see that, for each $k$,

$$
\text{span}\{A\bar{r}_{k-1}, \ldots, A^{m}r_{k-1}\} = \text{span} \mathcal{W}^{(k)}_m,
$$

notice that, by Eq. (7), $(-\alpha^{(k)}_0 \bar{r}_k + \alpha^{(k)}_0 \bar{r}_{k-1}) \in \text{span}\{\bar{w}^{(k)}_m\}$. Thus, given the representation $A$ of the operator $A$ in the canonical basis, Eq. (2) holds for each $k$, $k = 1, \ldots, q$.

To prove that the arbitrarily chosen set $\Lambda$ is the spectrum of $A$, let us consider the matrix $[A]_S$ of the
operator \( A \) in the basis \( S \):

\[
[A]_S = \begin{bmatrix}
0 & 0 & \cdots & \alpha_0^{(1)} & 0 & 0 & \cdots & \alpha_0^{(2)} & 0 & 0 & \cdots & \alpha_0^{(q+1)} & 0 & 0 & \cdots & \alpha_0^{(q+1)} \\
1 & 0 & \cdots & \alpha_1^{(1)} & 0 & 0 & \cdots & \alpha_1^{(2)} & 0 & 0 & \cdots & \alpha_1^{(q+1)} & 0 & 0 & \cdots & \alpha_1^{(q+1)} \\
0 & 1 & \cdots & \alpha_2^{(1)} & 0 & 0 & \cdots & \alpha_2^{(2)} & 0 & 0 & \cdots & \alpha_2^{(q+1)} & 0 & 0 & \cdots & \alpha_2^{(q+1)} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & \alpha_{m-1}^{(1)} & 0 & 0 & \cdots & \alpha_{m-1}^{(2)} & 0 & 0 & \cdots & \alpha_{m-1}^{(q+1)} & 0 & 0 & \cdots & \alpha_{m-1}^{(q+1)} \\
0 & 0 & \cdots & -\alpha_0^{(1)} & 0 & 0 & \cdots & -\alpha_0^{(2)} & 0 & 0 & \cdots & -\alpha_0^{(q+1)} & 0 & 0 & \cdots & -\alpha_0^{(q+1)} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & -\alpha_{q}^{(1)} & 0 & 0 & \cdots & -\alpha_{q}^{(2)} & 0 & 0 & \cdots & -\alpha_{q}^{(q+1)} & 0 & 0 & \cdots & -\alpha_{q}^{(q+1)} \\
0 & 0 & \cdots & -\alpha_{q+1}^{(1)} & 0 & 0 & \cdots & -\alpha_{q+1}^{(2)} & 0 & 0 & \cdots & -\alpha_{q+1}^{(q+1)} & 0 & 0 & \cdots & -\alpha_{q+1}^{(q+1)} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & -\alpha_{m}^{(1)} & 0 & 0 & \cdots & -\alpha_{m}^{(2)} & 0 & 0 & \cdots & -\alpha_{m}^{(q+1)} & 0 & 0 & \cdots & -\alpha_{m}^{(q+1)} \\
\end{bmatrix}
\]

The matrix \([A]_S\) has a block lower triangular structure, hence \([A]_S\)’s spectrum is the union of the eigenvalues of all diagonal blocks, which are the companion matrices corresponding to the sets \(\Lambda_k\) with characteristic polynomials defined in (13) and (14). Thus, the spectrum of \( A \) is \( \Lambda \).

\[\Box\]

### 2.4 Step 3: Conclusion of the proof of Theorem 2

Finally, we define \( A \) as the representation of the operator \( A \) in the canonical basis: \( \{e_1, e_2, \ldots, e_n\} \),

\[
A = S [A]_S S^{-1},
\]

where the square matrix \( S \) is formed by the vectors given in Eq. (12) written as columns and \([A]_S\) is defined by Eq. (16). The constructed matrix \( A \) provides the prescribed norms of residual vectors at the first \( q \) GMRES\((m)\) cycles when starting with \( r_0 \) and its spectrum is \( \Lambda \).

### 2.5 Difference with the work of Greenbaum, Pták, and Strakoš [12]

For the reader familiar with the work of Greenbaum, Pták, and Strakoš [12], it might be tempting to obtain the present result by pursuing the following scheme: fix \( r_0 \) and then consider the first restarted GMRES cycle as the initial part of a full GMRES run where the convergence is prescribed for the first \( m \) iterations (and arbitrarily set for the remaining \( n - m \) iterations). Then, similarly, given the starting residual vector \( r_1 \) provided by this first cycle, construct the next Krylov residual subspace which provides the desired convergence following the scheme of Greenbaum, Pták, and Strakoš [12]. Proceed identically for the remaining cycles. This approach, however, does not guarantee the linear independence of the set \( \mathfrak{F} \) and, hence, one meets the problem of defining the linear operator \( A \). These considerations were the reason for the assumption (7) on the residual reduction inside a cycle, which allowed to quite easily justify the linear independence of the set \( \mathfrak{F} \) and, as well, to control the spectrum.
3 Generating stagnating example of restarted GMRES

Theorem 3 handles the case for the decreasing positive sequence \( \{f(k)\}_{k=0}^{q} \). In this section, we are concerned with the stagnation case: when \( f(0) > f(1) > \cdots > f(s) > 0 \) and \( f(s+1) = \cdots = f(q) \).

**Theorem 3** Given a matrix order \( n \), a restart parameter \( m \) (\( m < n \)), a positive sequence \( \{f(k)\}_{k=0}^{q} \), which is either decreasing, or such that \( f(0) > f(1) > \cdots > f(s) > 0 \) and \( f(s+1) = \cdots = f(q) \), where \( q < n/m \), \( s < q \). There exists an \( n \)-by-\( n \) matrix \( A \) and a vector \( r_0 \) with \( \|r_0\| = f(0) \) such that \( \|r_k\| = f(k) \), \( k = 1, \ldots, q \), where \( r_k \) is the residual at cycle \( k \) of restarted GMRES with restart parameter \( m \) applied to the linear system \( Ax = b \), with initial residual \( r_0 = b - Ax_0 \). Moreover, the matrix \( A \) can be chosen to have any desired eigenvalues.

**Proof.** The decreasing convergence case is handled by Theorem 2. Therefore, we only need to construct a matrix \( A \) with a spectrum \( \Lambda \) and an initial residual vector \( r_0 \), \( \|r_0\| = f(0) \) for which restarted GMRES stagnates at cycle \( s+1 \) while \( \|r_1\| = f(1) > \cdots > \|r_s\| = f(s) \), \( s < q \).

By Lemma 1 given the initial residual vector \( r_0 \), \( \|r_0\| = f(0) \), we can construct residual vectors \( r_k \) with the prescribed norms \( f(k) \), and orthonormal sets \( W_m(k) \), \( k = 1, \ldots, s \), such that the set

\[
\{r_0, W_m(1), \ldots, r_{s-1}, W_m(s), r_s\}
\]

is linearly independent. In order to enforce stagnation at the \( (s+1) \)-st GMRES(\( m \)) cycle, we want the next orthonormal set \( W_m(s+1) \) to be orthogonal to the residual vector \( r_s \). (See Eq. (6) or (7).) Thus, following the pattern in Lemma 1 we choose \( W_m(s+1) \) from the orthogonal complement of the set \( \{W_m(1), \ldots, W_m(s), r_s\} \), and append \( W_m(s+1) \) to the set \( \{W_m(1), \ldots, W_m(s), r_s\} \), thus obtaining the linearly independent set

\[
\{r_0, W_m(1), \ldots, r_{s-1}, W_m(s), r_s, W_m(s+1)\}.
\]

At this point, if we followed the proof of Lemma 1 we would append the new residual vector \( r_{s+1} \) to the set \( \{W_m(1), \ldots, W_m(s), r_s\} \). Since \( r_s = r_{s+1} \), this would result in the loss of the linear independence of our set. Instead, we would like to expand the set \( \{W_m(1), \ldots, W_m(s), r_s\} \) by some vector that will not spoil the linear independence and will allow for a proper definition of the operator \( A \) at the second step of the proof. To fulfill this task, we choose this vector to be \( w_m(s+1) + r_s \) and append it to \( \{W_m(1), \ldots, W_m(s), r_s\} \). We obtain the set

\[
\{r_0, W_m(1), \ldots, r_{s-1}, W_m(s), r_s, W_m(s+1), w_m(s+1) + r_s\},
\]

which is linearly independent, since the vector \( w_m(s+1) + r_s \) has the component \( w_m(s+1) \) from the orthogonal complement of \( \{W_m(1), \ldots, W_m(s), r_s\} \) and hence cannot be represented as a linear combination of vectors in this set.

Expanding \( \{W_m(1), \ldots, W_m(s), r_s\} \) with vectors \( \hat{S} = \{\hat{s}_1, \ldots, \hat{s}_t\} \), we finally construct the basis of \( \mathbb{C}^n \):

\[
\hat{S} = \{r_0, W_m(1), \ldots, r_{s-1}, W_m(s), r_s, W_m(s+1), w_m(s+1) + r_s, \hat{s}_1, \ldots, \hat{s}_t\},
\]

where \( t = n - m(s+1) - 1 \).

Now, following the previously described pattern, we need to define an operator \( A \) with a prescribed spectrum \( \Lambda \), represented by the matrix \( A \) in the canonical basis, such that Eq. (2) is satisfied for \( k = 1, \ldots, s + 1 \). We split \( \Lambda \) into the disjoint subsets \( \Lambda = \{\Lambda_1, \Lambda_2, \ldots, \Lambda_{s+1}, \Lambda_{s+2}\} \), so that each \( \Lambda_k \) consists of \( m \) sequential elements of \( \Lambda \), \( k = 1, \ldots, s + 1 \), while the rest \( n - m(s+1) \) elements are included into \( \Lambda_{s+2} \). Similarly to (13)–(14), for each \( k \), we introduce the polynomials

\[
p_k(x) = x^m - \sum_{j=0}^{m-1} \alpha_j^{(k)} x^j, \quad k = 1, \ldots, s + 1;
\]

\[
p_{s+2}(x) = x^{t+1} - \sum_{j=0}^{t} \alpha_j^{(s+2)} x^j, \quad t = n - m(s+1) - 1;
\]

where the roots of each polynomial are in the respective set \( \Lambda_k \), \( k = 1, \ldots, s + 2 \).
Similarly to [13], we define the operator $\mathcal{A}$ as following:

$\mathcal{A}r_{k-1} = w^{(k)}_1,$
$\mathcal{A}w^{(k)}_1 = w^{(k)}_2,$
\[\vdots\]
$\mathcal{A}w^{(k)}_{m-2} = w^{(k)}_{m-1},$
$\mathcal{A}w^{(k)}_{m-1} = -\alpha^{(k)}_0 r_k + \alpha^{(k)}_0 r_{k-1} + \alpha^{(k)}_1 w^{(k)}_1 + \cdots + \alpha^{(k)}_{m-1} w^{(k)}_{m-1}, k = 1, \ldots, s;$
$\mathcal{A}r_s = w^{(s+1)}_1,$
$\mathcal{A}w^{(s+1)}_1 = w^{(s+1)}_2,$
\[\vdots\]
$\mathcal{A}w^{(s+1)}_{m-2} = w^{(s+1)}_{m-1},$
$\mathcal{A}w^{(s+1)}_{m-1} = -\alpha^{(s+1)}_0 (w^{(s+1)}_m + r_s) + \alpha^{(s+1)}_0 r_s + \alpha^{(s+1)}_1 w^{(s+1)}_1 + \cdots + \alpha^{(s+1)}_{m-1} w^{(s+1)}_{m-1},$
$\mathcal{A}(w^{(s+1)}_m + r_s) = \hat{s}_1,$
$\mathcal{A}\hat{s}_1 = \hat{s}_2,$
\[\vdots\]
$\mathcal{A}\hat{s}_{t-1} = \hat{s}_t,$
$\mathcal{A}\hat{s}_t = \alpha^{(s+2)}_0 (w^{(s+1)}_m + r_s) + \alpha^{(s+2)}_1 \hat{s}_1 + \cdots + \alpha^{(s+2)}_t \hat{s}_t,$

where $\alpha^{(k)}_i$'s are the coefficients of polynomials (22) and (23). From the definition (24) of the operator $\mathcal{A}$, one can observe that for each $k, j = 1, \ldots, s + 1$, the set

$$\text{span}\{\mathcal{A}r_{k-1}, \ldots, \mathcal{A}r_{k-1}\} = \text{span} \{W^{(j)}_m\}, \ j = 1, \ldots, m.$$ 

Thus, given the representation $A$ of the operator $\mathcal{A}$ in the canonical basis, we can guarantee that Eq. (2) holds for each $k, j = 1, \ldots, s + 1$.

Similarly to Eq. (16), the structure of the matrix $[A]_\mathcal{S}$ of the operator $\mathcal{A}$ in the basis $\mathcal{S}$ will be block lower triangular with each diagonal block being the companion matrix for the corresponding subset $\Lambda_k$ of $A$'s eigenvalues, where characteristic polynomials are defined by (22)–(23), and $-\alpha^{(k)}_0$'s being subdiagonal elements. The desired matrix $A$ is then obtained by similarity transformation

$$A = \hat{S} [A]_\mathcal{S} \hat{S}^{-1},$$

where the square matrix $\hat{S}$ is formed by the set of vectors (21) written as columns.

\[\Box\]

4 Restarted GMRES with variable restart parameter

The result given by Theorem 3 generalizes to the case when the restart parameter $m$ is not fixed, but varies over the successive cycles with a priori prescribed restart parameters $m_k$ for the corresponding GMRES($m_k$) cycles.

Corollary 1 Given a matrix order $n$, a sequence $\{m_k\}_{k=1}^q$ of restart parameters with $1 \leq m_k \leq n - 1$, $\sum_{k=1}^s m_k < n$, and a positive sequence $\{f(k)\}_{k=0}^q$, which is either decreasing, or such that $f(0) > f(1) > \cdots > f(s) > 0$ and $f(s) = f(s + 1) = \cdots = f(q)$, where $s < q$. There exits an $n$-by-$n$ matrix $A$ and a vector $r_0$ with $\|r_0\| = f(0)$ such that $\|r_k\| = f(k)$, $k = 1, \ldots, q$, where $r_k$ is the residual at cycle $k$ of restarted GMRES with a variable restart parameter $m_k$ applied to the linear system $Ax = b$, with initial residual $r_0 = b - Ax_0$. Moreover, the matrix $A$ can be chosen to have any desired eigenvalues.
Proof The proof follows directly from Lemma 1, Lemma 2 and Theorem 2. Note that the constructed operator $A$ will have block lower triangular matrices with block sizes $m_k$ (instead of $m$).

5 Generating non-convergent examples

When constructing a matrix $A$ and an initial residual vector $r_0$ which provide the prescribed decreasing cycle-convergence generated by GMRES($m$), we note that from the last line of the definition (14) of the operator $A$ we obtain

$$r_q \in AK_{l+1}(A, r_q),$$

where $A$ is the representation of the operator $A$ in the canonical basis and $t = n - mq - 1$. This equality implies that at the end of the $(q + 1)$-st cycle GMRES($m$) converges to the exact solution of Eq. (1), i.e. $r_{q+1} = 0$. This fact might seem unnatural and undesirable, e.g., for constructing academic examples. The “drawback”, however, can be easily fixed by a slight correction of the basis $S$ – somewhat similarly to how we handled the stagnation case in Theorem 3.

Given residuals $r_k$ and orthonormal sets $W_{m}^{(k)}$ constructed according to Lemma 1 instead of considering the set $S$, we consider the following basis of $\mathbb{C}^n$:

$$\tilde{S} = \{ r_0, w_1^{(1)}, \ldots, w_{m-1}^{(1)}, r_q^{(1)}, \ldots, w_{m-1}^{(q)}, r_{m-1}^{(q+1)} + \gamma r_q, \tilde{s}_1, \ldots, \tilde{s}_t \},$$

where $\gamma \neq -1$. Here we substituted the basis vector $r_q$ in Eq. (12) by $r_q + \gamma q r_q - 1$. The vector $r_q + \gamma q r_q - 1$ cannot be represented as a linear combination of other vectors in $\tilde{S}$, since it contains the component $r_q$, which is not represented by these vectors. Hence, $\tilde{S}$ is indeed a basis of $\mathbb{C}^n$. Thus we can define the operator $A$ by its action on $\tilde{S}$:

$$A r_{k-1} = w_1^{(k)},$$

$$A w_1^{(k)} = w_2^{(k)},$$

$$\vdots$$

$$A w_{m-2}^{(k)} = w_{m-1}^{(k)},$$

$$A w_{m-1}^{(k)} = -\alpha_0^{(k)} r_k + \alpha_0^{(k)} r_{k-1} + \alpha_1^{(k)} w_1^{(k)} + \cdots + \alpha_{m-1}^{(k)} w_{m-1}^{(k)}, \quad k = 1, \ldots, q - 1;$$

$$A r_q^{(q)} = w_1^{(q)},$$

$$A w_1^{(q)} = w_2^{(q)},$$

$$\vdots$$

$$A w_{m-2}^{(q)} = w_{m-1}^{(q)},$$

$$A w_{m-1}^{(q)} = -\alpha_0^{(q)} \frac{r_{q} + \gamma q r_q - 1}{1 + \gamma} + \alpha_0^{(q)} r_{q-1} + \alpha_1^{(q)} w_1^{(q)} + \cdots + \alpha_{m-1}^{(q)} w_{m-1}^{(q)},$$

$$A(r_q + \gamma q r_q - 1) = \tilde{s}_1,$$

$$\tilde{A} s_1 = \tilde{s}_2,$$

$$\vdots$$

$$\tilde{A} s_{t-1} = \tilde{s}_t,$$

$$\tilde{A} s_t = \alpha_0^{(q+1)}(r_{q} + \gamma q r_q - 1) + \alpha_1^{(q+1)} \tilde{s}_1 + \cdots + \alpha_t^{(q+1)} \tilde{s}_t,$$

where $\alpha_j^{(k)}$'s are the coefficients of the corresponding characteristic polynomials (13) and (14). The fact that the operator $A$ produces the correct Krylov residual subspace at the cycle $q$, i.e.,

$$\text{span}\{A r_{q-1}, \ldots, A^m r_q - 1\} = \text{span} W_{m}^{(q)},$$
can be observed from the following equalities:

\[ A w^{(q)}_{m-1} = \frac{-\alpha_0^{(q)}}{1 + \gamma} (r_q + \gamma r_{q-1}) + \alpha_0^{(q)} w^{(q)}_1 + \cdots + \alpha_m^{(q)} w^{(q)}_{m-1} \]

\[ = \frac{-\alpha_0^{(q)}}{1 + \gamma} (r_q - r_{q-1} + (1 + \gamma) r_{q-1}) + \alpha_0^{(q)} w^{(q)}_1 + \cdots + \alpha_m^{(q)} w^{(q)}_{m-1} \]

\[ = \frac{-\alpha_0^{(q)}}{1 + \gamma} (r_q - r_{q-1}) + \alpha_1^{(q)} w^{(q)}_1 + \cdots + \alpha_m^{(q)} w^{(q)}_{m-1}, \]

where, by Eq. (26), \( A w^{(q)}_{m-1} = A^m r_{q-1} \) and, by Eq. (7), \( (r_q - r_{q-1}) \in \text{span}\{ w^{(q)}_m \} \).

The matrix \( [A]_S \) of the operator \( A \), defined by Eq. (26), in the basis \( S \) is identical to Eq. (16) with the only change of the subdiagonal element \( -\alpha_0^{(q)} \) to \( \frac{-\alpha_0^{(q)}}{1 + \gamma} \), \( \gamma \neq -1 \). Hence, \( A \) has the desired spectrum \( \Lambda \).

Thus, finally, according to Eq. (26),

\[ r_q \in \mathcal{K}_{t+1} (A, r_q) + \mathcal{K}_{t+2} (A, r_{q-1}) \]

providing that \( r_{q+1} \) is nonzero.

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