On investigating GMRES convergence using unitary matrices

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Abstract

For a given matrix A and right-hand side b, this paper investigates unitary matrices generating, with some right-hand sides c, the same GMRES residual norms as the pair (A, b). We give characterizations of this class of unitary matrices and point out the relationship with Krylov subspaces and Krylov residual subspaces for the pair (A, b). We investigate the eigenvalues of these unitary matrices in relation to the convergence behavior of GMRES for the pair (A, b) and describe the indispensable role of the eigenvector information. We conclude with a formula for the GMRES residual norms generated by a normal matrix B in terms of its eigenvalues and components of the right-hand side c in the eigenvector basis.

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GMRES convergence, unitary matrices, unitary spectra, normal matrices, Krylov residual subspace, Schur parameters
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1. Introduction

In this paper we consider the convergence behavior of the GMRES method for solving linear systems

$$Ax = b$$

with (generally complex) square matrices A of order n and right-hand sides b; for a detailed description of this popular Krylov subspace method see [1] or [2]. With no loss of generality, we consider zero initial guess $x_0 = 0$. The kth GMRES iterate is the vector x_k in the kth Krylov subspace which minimizes the residual norm, that is

$$x_k = \arg \min_{x \in \mathcal{K}_k(A,b)} \|b - Ax\|, \qquad \mathcal{K}_k(A,b) \equiv \text{span}\{b,\, Ab,\, \ldots,\, A^{k-1}b\}. \quad (1)$$

It follows that the kth residual vector $r_k = b - Ax_k$ is the difference between b and its orthogonal projection onto the Krylov *residual* subspace $A\mathcal{K}_k(A,b)$. A standard convergence bound for the kth residual norm with diagonalizable A is

$$\frac{\|r_k\|}{\|b\|} \leq \kappa(Z) \min_{p \in \Pi_k} \max_{i=1,\ldots,n} |p_k(\lambda_i)|, \quad (2)$$

where A has the spectral decomposition $A = Z\Lambda Z^{-1}$, $\Lambda = \text{diag}\,(\lambda_1, \ldots, \lambda_n)$, $\kappa(Z)$ is the condition number of the eigenvector matrix and Π_k is the set of polynomials of degree k with the value one at the origin (see, e.g., [2]). For Hermitian matrices, convergence of Krylov subspace methods like Conjugate Gradient or MINRES is very strongly linked with the eigenvalue distribution. For instance, the values these methods minimize (some norm of the error or residual vector) can be bounded with the same bound as in (2) where $\kappa(Z) = 1$. This bound then depends on the spectrum only and, concerning the envelope of all possible convergence curves for matrices A having the given spectrum, it is sharp [3], i.e., for every k there exists a right-hand side (depending on k) such that equality holds in (2). However, it has been known for some time that eigenvalues alone cannot explain GMRES convergence for non-Hermitian and, more specifically, for non-normal matrices. This was first shown in the 1994 paper [4], in which the authors studied the matrices B that generate the same Krylov residual space as the one given by the pair (A, b), that is

$$B\mathcal{K}_k(B,b) = A\mathcal{K}_k(A,b), \;\; k = 1, 2, \ldots, n.$$

Then GMRES applied to (B, b) yields the same convergence history (with respect to residual norms) as GMRES applied to (A, b). Matrices B with this property will be called GMRES (A, b)-equivalent matrices. They can be characterized as follows (we assume for simplicity of notation, that GMRES applied to A, b does not terminate until the step n, i.e., $\dim(\mathcal{K}_n(A,b)) = n$).

Theorem 1 (Theorem 1 of [4]). *Let W be a unitary matrix whose first k columns give a basis of $A\mathcal{K}_k(A, b)$ for all k with $1 \leq k \leq n$ and let $\mathcal{H}$ be an unreduced upper Hessenberg matrix such that $AW = W\mathcal{H}$. Then, the following assertions are equivalent:*

1- B is GMRES(A, b)-equivalent,

2- $B = W\tilde{R}\mathcal{H}W^*$, where $\tilde{R}$ is any nonsingular upper triangular matrix.

Among other results, it is shown in [4] that the spectrum of B can consist of arbitrary nonzero values. In [5] this was extended by proving the fact that any nonincreasing sequence of residual norms can be generated by GMRES and [6] closed this series of papers with a full parametrization of the class of matrices and right-hand sides giving prescribed convergence history while the system matrix has prescribed nonzero spectrum; for a survey we refer to [7, Section 5.7]. In [8] a parametrization was given of the class of matrices and right-hand sides generating, in addition to prescribed residual norms and eigenvalues, prescribed Ritz values in all iterations.

While all these results show that spectral information only can be misleading when explaining GMRES convergence behavior with general matrices, GMRES convergence *is* bounded using the eigenvalue distribution when it is applied to normal matrices in view of (2). More strongly, GMRES convergence is for normal matrices *determined* by the approximation problem

$$\|r_k\| = \min_{p \in \Pi_k} \|p\,(\Lambda) Z^* b\|. \tag{3}$$

On page 13 of [4] the authors wrote, with respect to Theorem 1: "If, for each vector b, we can find a matrix B of the given form, for which we can analyze the behavior of the GMRES method applied to B, then we can also analyze the behavior of the GMRES method applied to A. Since the behavior of the GMRES method for normal matrices is well-understood in terms of the eigenvalues of the matrix, it is desirable to find an upper triangular matrix $\tilde{R}$ such that $\tilde{R}\mathcal{H}$ is normal." It was shown subsequently in [4] that $\tilde{R}$ can always be chosen such that $\tilde{R}\mathcal{H}$ is normal and even unitary, and under some assumptions such that $\tilde{R}\mathcal{H}$ is Hermitian positive definite or just Hermitian. In general, however, no simple properties of A were found which are related to the spectral properties of a GMRES$\,(A, b)$-equivalent normal matrix.

Two papers, both published in 2000, analyzed the eigenvalues of particular unitary GMRES$\,(A, b)$-equivalent matrices and studied in detail the relation with GMRES convergence. In [9], Liesen used QR and RQ factorizations of the matrix $\mathcal{H}$ to obtain bounds for the residual norms in terms of the largest gap in the spectrum of the Q factors on the unit circle. He showed, among other things, that a large maximum gap in the spectrum of the Q factor in an RQ factorization $\mathcal{H} = R\mathcal{Q}$ implies fast GMRES convergence; see also his Ph.D. Thesis [10, Section 5]. In [11], Knizhnerman considered $\mathcal{H}$ to be a possibly infinite dimensional bounded operator and showed an inverse result, namely that for finite operators (matrices), fast GMRES convergence implies a large gap in the spectrum of $\mathcal{Q}$ in a certain RQ factorization of $\mathcal{H}$. It was also shown that the entries of this particular $\mathcal{Q}$ can be expressed in terms of the residual norms only [11, Section 6.1].

The goal of this paper is to further explore how and to what extent GMRES convergence can be explained using unitary GMRES (A, b)-equivalent pairs. With a unitary GMRES (A, b)-equivalent pair (B, c) we mean a matrix B with a right-hand side c which generate the same convergence history as (A, b) where B is unitary and c is not necessarily equal to b. We will characterize such pairs and investigate their properties. Unlike in [4], we will not consider the unitary matrix W in $B = W\tilde{R}\mathcal{H}W^*$ (see Theorem 1) merely an unimportant change of variables matrix, whose influence is not taken into account when analyzing the spectrum of B. Our investigation will rely on the fact that the first k columns of W form a basis of $A\mathcal{K}_k(A, b)$, $1 \leq k \leq n$. We show that all unitary GMRES (A, b)-equivalent matrices B can be constructed from W and from a unitary matrix V whose first k orthogonal columns form bases of $\mathcal{K}_k(A, b)$, $1 \leq k \leq n$. Since V and W depend strongly on the interplay between A and b, our goal cannot be in relating GMRES convergence to some simple properties of A only. Instead, we will describe how both the eigenvalues of B and components of c in the eigenvector basis of B determine the convergence curve. This will be based on a new explicit expression for the kth residual norm generated by a normal matrix.

The paper is organized as follows. Section 2 characterizes GMRES (A, b)-equivalent matrices B and pairs (B, c), where B is unitary, and it explains their relationship to the Krylov subspaces and Krylov residual subspaces produced by A and b. In this section it is also shown that the eigenvectors of B play a substantial role in the description of convergence for GMRES applied to (A, b). Section 3 contains the derivation of a formula for the kth GMRES residual norm in terms of the eigenvalues, eigenvectors and the right-hand side when GMRES is applied to a normal matrix. These quantities can be useful to gain some insight in the convergence for (A, b) with the help of a

GMRES (A, b)-equivalent pair where the matrix is normal and, in particular, unitary.

Throughout the paper we will assume, as mentioned above, that GMRES does not terminate until the last step n. Hence, the Krylov subspaces are of full dimension and their orthogonal bases constructed using the Gram-Schmidt algorithm are well defined. We also assume the zero initial guess in all applications of GMRES. For simplicity we normalize the right-hand side b such that $\|b\| = 1$. We will use repeatedly the fact that GMRES residual norm convergence is unitarily invariant in the sense that, U being any unitary matrix, the pair (U^*AU, U^*b) generates the same residual norms as (A, b). With e_i we will denote the ith column of the identity matrix (of appropriate order). With "the subdiagonal" and "subdiagonal entries" of an upper Hessenberg matrix we will mean the (entries on the) first subdiagonal under the main diagonal. Hessenberg matrices with a real positive subdiagonal will be denoted with a plus as lower index, for example H_+.

2. Unitary GMRES (A, b)-equivalent pairs

In this section we characterize pairs (B, c) which yield the same GMRES convergence history as (A, b) with B unitary and c not necessarily equal to b. We describe their relationship to the Krylov subspaces and Krylov residual subspaces generated by (A, b) and study the influence of the spectrum of B on the convergence history for (A, b).

2.1. Unitary GMRES (A, b)-equivalent matrices

First let us consider the case where $c = b$. Here is a characterization of the class of all unitary GMRES (A, b)-equivalent matrices.

Proposition 2. *Let W be a unitary matrix whose first k columns give a basis of $A\mathcal{K}_k(A, b)$ for $1 \leq k \leq n$, let $\mathcal{H}$ be an unreduced upper Hessenberg matrix such that $AW = W\mathcal{H}$ and let $\mathcal{H} = R\mathcal{Q}$ be an RQ factorization of $\mathcal{H}$. Then, the following assertions are equivalent:*

1- B is unitary and GMRES (A, b)-equivalent,

2- $B = WD_1\mathcal{Q}W^*$, where D_1 is a diagonal unitary matrix.

PROOF. Any RQ factorization of $\mathcal{H}$ has the form $\mathcal{H} = (RD_0^{-1})(D_0\mathcal{Q})$, where D_0 is a diagonal unitary matrix. Thus, with the notation of Theorem 1, B is unitary if and only if $B = W(\tilde{R}RD_0^{-1})(D_0\mathcal{Q})W^*$ is unitary, which is true if and only if $\tilde{R}R$ is unitary. This holds if and only if $\tilde{R} = D_1R^{-1}$ for a diagonal unitary matrix D_1, giving $B = WD_1D_0^{-1}D_0\mathcal{Q}W^* = WD_1\mathcal{Q}W^*$. $\square$

Thus *all* unitary GMRES (A, b)-equivalent matrices are of the form $B = W\mathcal{Q}W^*$ where $\mathcal{Q}$ is the unitary factor of an RQ decomposition of $\mathcal{H}$.

Note that the Hessenberg matrix $\mathcal{H}$ is not the Hessenberg matrix generated in a standard implementation of GMRES where an orthogonal basis of $\mathcal{K}_n(A, b)$ is built. $\mathcal{H}$ results from building an orthogonal basis of $A\mathcal{K}_n(A, b)$ by starting the Arnoldi process with the vector $Ab/\|Ab\|$. This is done, for example, in the Walker-Zhou implementation of GMRES [12]. In a standard implementation of GMRES, one constructs the unitary matrix $\hat{V}$ whose first k columns span the Krylov space $\mathcal{K}_k(A, b)$ for all $1 \leq k \leq n$ and which is the result of the Arnoldi orthogonalization process applied to (A, b). More precisely, the unitary $\hat{V}$ satisfies

$$A\hat{V} = \hat{V}H_+, \qquad \hat{V}e_1 = b, \tag{4}$$

for an unreduced upper Hessenberg matrix H_+ with positive subdiagonal entries. Consider the unique QR decomposition

$$H_+ = Q^+\mathcal{R} \tag{5}$$

such that Q^+ is a unitary upper Hessenberg matrix with a real positive first row; see [13]. The entries of the matrix $\mathcal{Q}$ from an RQ decomposition of $\mathcal{H}$ were given in terms of the GMRES residual norms in equation (6.1) of [11]. Interestingly enough, the moduli of the entries of Q^+ and $\mathcal{Q}$ coincide. In order to show this, we need the following lemma. For real matrices, it was also proved in [13, Theorem 3.1].

Lemma 3. *Let W be a unitary matrix whose first k columns give a basis of $A\mathcal{K}_k(A, b)$ for $1 \leq k \leq n$ and let $\hat{V}$ be the unitary matrix in (4). If Q^+ is the unitary factor in the QR factorization (5) of H_+, then*

$$Q^+ = \hat{V}^*WD_2,$$

where D_2 is a diagonal unitary matrix.

PROOF. Because the first k columns of W form a basis of $A\mathcal{K}_k(A,b)$, $1 \leq k \leq n$, we can write

$$A\hat{V} = W\hat{R}$$

for some nonsingular upper triangular matrix $\hat{R}$. Then from $A\hat{V} = \hat{V}H_+ = W\hat{R}$ we have the QR decomposition

$$H_+ = (\hat{V}^*W)\hat{R}.$$

Hence, for the properly chosen diagonal unitary matrix D_2, $Q^+ = \hat{V}^*WD_2$ has its first row real and positive. $\square$

Corollary 4. *Let Q^+ be the unitary factor in the QR factorization (5) and let $\mathcal{Q}$ be the unitary factor of an RQ decomposition of $\mathcal{H}$. Then*

$$\mathcal{Q} = D_3^*Q^+D_2^*$$

where D_2 is the matrix of Lemma 3 and D_3 is a diagonal unitary matrix.

PROOF. From (4) and Lemma 3 we have

$$AWD_2(Q^+)^* = WD_2(Q^+)^*H_+,$$

which implies

$$W^*AW = \mathcal{H} = D_2(Q^+)^*H_+Q^+D_2^*.$$

Hence we have the RQ decomposition

$$\mathcal{H} = D_2(Q^+)^*(Q^+\mathcal{R})Q^+D_2^* = (D_2\mathcal{R})(Q^+D_2^*).$$

Therefore, $\mathcal{Q}$ is of the form $\mathcal{Q} = D_3^*Q^+D_2^*$ for some diagonal unitary matrix D_3. $\square$

Lemma 3 enables another characterization of unitary GMRES (A,b)-equivalent matrices; cf. Proposition 2.

Theorem 5. *The following assertions are equivalent:*

1- B is unitary and GMRES(A,b)-equivalent, *2- $B = WV^*$, where V is a unitary matrix whose first k columns give a basis of $\mathcal{K}_k(A,b)$ and W is a unitary matrix whose first k columns give a basis of $A\mathcal{K}_n(A,b)$ for $1 \le k \le n$.*

Proof. Because of Proposition 2, if B is unitary and GMRES (A,b)-equivalent, then B is of the form

$$B = \hat{W} D_1 \mathcal{Q} \hat{W}^*,$$

where the columns of $\hat{W}$ are an orthonormal basis of $A\mathcal{K}_n(A,b)$. Using Lemma 3 and Corollary 4, we obtain

$$B = \hat{W} D_1 \mathcal{Q} \hat{W}^* = \hat{W} D_1 D_3^* Q^+ D_2^* \hat{W}^* = \hat{W} D_1 D_3^* \hat{V}^* \hat{W} \hat{W}^* = \hat{W} D_1 D_3^* \hat{V}^*.$$

Putting $V = \hat{V} D_3$ and $W = \hat{W} D_1$ gives the first implication. Now let $B = WV^*$. Then with Lemma 3, for some diagonal unitary matrix D_4,

$$B = W(V^* W) W^* = W(D_4 \hat{V}^* W) W^* = W(D_4 Q^+ D_2^*) W^*$$

and with Corollary 4,

$$B = W(D_4 Q^+ D_2^*) W^* = W(D_4 D_3 \mathcal{Q} D_2 D_2^*) W^* = W(D_4 D_3 \mathcal{Q}) W^*.$$

This yields the second implication if we use Proposition 2. □

This theorem shows how closely unitary GMRES (A,b)-equivalent matrices are related to the Krylov subspaces $\mathcal{K}_k(A,b)$ and the Krylov residual subspaces $A\mathcal{K}_k(A,b)$ for $1 \le k \le n$. These subspaces, and therefore also the matrices V and W, depend strongly on the interplay between A and b. Linking the properties of unitary GMRES (A,b)-equivalent matrices (like spectral properties) to some simple properties of A only is therefore rather complicated.

With the help of Theorem 5 we can characterize the eigenvalues of unitary GMRES (A,b)-equivalent matrices in terms of the Krylov subspaces $\mathcal{K}_k(A,b)$ and the Krylov residual subspaces $A\mathcal{K}_k(A,b)$, $1 \le k \le n$. GMRES convergence for (A,b) is bounded by these eigenvalues in the following sense.

Corollary 6. *Using the notation of Theorem 5, the GMRES residual norms for the pair (A,b) are bounded as*

$$\frac{\|r_k\|}{\|b\|} \le \min_{p \in \Pi_k} \max_{i=1,\ldots,n} |p_k(\mu_i)|, \tag{6}$$

with $\mu_1, \ldots, \mu_n$ being the eigenvalues in the generalized eigenvalue problem

$$V^*x = \mu W^*x. \tag{7}$$

It is worth noticing that in (6) the polynomials are evaluated at points which depend through V and W in (7) on the right-hand side b.

2.2. Unitary GMRES(A, b)-equivalent pairs

Now we come to unitary matrices that give the same residual norm convergence curve as (A, b) with a right-hand side possibly different from b. Our goal will be to characterize the set of all pairs (B, c) with these properties. *Some* pairs are obtained simply by using the fact that GMRES convergence is unitarily invariant. For example, let us consider a unitary GMRES(A, b)-equivalent matrix $B = WV^*$ defined in Theorem 5 and let us define S by interchanging V and W, i.e.

$$S = V^*W. \tag{8}$$

Since GMRES convergence is unitarily invariant, the pair $(W^*BW, W^*b) = (V^*W, W^*b) = (S, W^*b)$ gives also the same residual norm convergence curve. We can find a GMRES(A, b)-equivalent pair with the same unitary system matrix S but a *different* right-hand side: Using the unitary equivalence $(B, b) = (V^*WV^*V, V^*b) = (S, e_1)$ we obtain the GMRES(A, b)-equivalent pair (S, e_1). Since B is normal, we have $B = Z\Delta Z^*$ where Z is unitary and Δ is the diagonal matrix containing the eigenvalues of B. Therefore yet another GMRES(A, b)-equivalent pair is (Δ, Z^*b).

We next give a parametrization of all GMRES(A, b)-equivalent pairs with a unitary system matrix. For our result we will exploit the relationship between unitary upper Hessenberg matrices with real positive subdiagonals and the so-called Schur parameters. This relationship is briefly outlined below.

2.2.1. Unitary Hessenberg matrices and Schur parameters

Any unitary upper Hessenberg matrix of order n with positive subdiagonal entries can be uniquely parametrized by n complex parameters γ_k such that $|\gamma_k| < 1$, $k = 1, \ldots, n-1$ and $|\gamma_n| = 1$, see, e.g., [14, 15, 16, 17, 18, 19] or, for a reference from functional analysis, [20, Section 4.1] where the parametrization is named *GGT representation* (after Geronimus, Gragg, and Teplzaev). We will denote such unitary upper Hessenberg matrices with Q_+ (not to be confounded with the unitary upper Hessenberg matrices Q^+ in (5) which have a positive first row but do not necessarily have a positive subdiagonal). The γ_k's are called Schur parameters (this term was introduced in [14]). They are also known as partial correlation coefficients in statistics and reflection coefficients in signal processing. It is useful to introduce the so-called complementary Schur parameters σ_k, $k = 1, \ldots, n-1$ which are real and positive such that $\sigma_k = \sqrt{1 - |\gamma_k|^2}$. The matrix Q_+ can be written as the product

$$Q_+ = G_1(\gamma_1)\, G_2(\gamma_2) \cdots G_{n-1}(\gamma_{n-1})\, \tilde{G}_n(\gamma_n),$$

where

$$G_k(\gamma_k) = \operatorname{diag}\left(I_{k-1}, \begin{bmatrix} -\gamma_k & \sigma_k \\ \sigma_k & \overline{\gamma_k} \end{bmatrix}, I_{n-k-1} \right), \qquad \tilde{G}_n(\gamma_n) = \operatorname{diag}(I_{n-1}, -\gamma_n), \tag{9}$$

and the nonzero entries of Q_+ are given by

$$q_{k+1,k} = \sigma_j, \quad q_{j,k} = -\overline{\gamma_{j-1}}\sigma_j\sigma_{j+1}\cdots\sigma_{k-1}\gamma_k,\ 1 \le j \le k. \tag{10}$$

This means that the matrix Q_+ has the following form (see [18]),

$$Q_+ = \begin{bmatrix} -\gamma_1 & -\sigma_1\gamma_2 & \cdots & \cdots & -\sigma_1\cdots\sigma_{k-1}\gamma_k & \cdots & -\sigma_1\cdots\sigma_{n-1}\gamma_n \\ \sigma_1 & -\overline{\gamma_1}\gamma_2 & \cdots & \cdots & -\overline{\gamma_1}\sigma_2\cdots\sigma_{k-1}\gamma_k & \cdots & -\overline{\gamma_1}\sigma_2\cdots\sigma_{n-1}\gamma_n \\ & \sigma_2 & -\overline{\gamma_2}\gamma_3 & \cdots & \vdots & \cdots & -\overline{\gamma_2}\sigma_3\cdots\sigma_{n-1}\gamma_n \\ & & \ddots & \ddots & & & \vdots \\ & & & \sigma_{k-1} & -\overline{\gamma_{k-1}}\gamma_k & \cdots & -\overline{\gamma_{k-1}}\sigma_k\cdots\sigma_{n-1}\gamma_n \\ & & & & & & \vdots \\ & & & & \ddots & & \\ & & & & & \sigma_{n-1} & -\overline{\gamma_{n-1}}\gamma_n \end{bmatrix}.$$

Conversely, if we know Q_+, then the Schur parameters and the complementary Schur parameters are given by

$$\gamma_k = -\frac{q_{1,k}}{\sigma_1\cdots\sigma_{k-1}},\ 1 \le k \le n, \qquad \sigma_k = q_{k+1,k},\ 1 \le k < n, \tag{11}$$

i.e., there is a one-to-one correspondence between Schur parameters and unitary upper Hessenberg matrices with positive subdiagonal entries.

We also mention the relationship of Schur parameters with Szegö polynomials. If Q_k is the leading (in general not unitary) principal submatrix of Q_+, then

$$\psi_k(\lambda) = \det(\lambda I - Q_k),$$

is the kth Szegö polynomial for $1 \leq k \leq n$ [21, Chapter XI]. Szegö polynomials can be computed from a recurrence whose coefficients are the Schur parameters.

2.2.2. GMRES residual norms and Schur parameters

The matrices $G_k(\gamma_k)$ in (9) remind us of Givens rotations used in the standard GMRES implementation (see, e.g., [1]). The Arnoldi process applied to the pair (A, b) generates the upper Hessenberg matrix H_+ in (4) (this matrix is, in general, not unitary). Instead of the QR decomposition (5) we can consider $H_+ = Q_+ \hat{R}$ where

$$\begin{aligned} Q_+^* &= F_1(c_1)\, F_2(c_2) \cdots F_{n-1}(c_{n-1}), \\ F_k(c_k) &= \operatorname{diag}\left(I_{k-1}, \begin{bmatrix} -\overline{c}_k & s_k \\ s_k & c_k \end{bmatrix}, I_{n-k-1} \right), \end{aligned}$$

with Givens rotation parameters c_k and $s_k > 0$ satisfying $|c_k|^2 + |s_k|^2 = 1$. With this choice Q_+ has positive subdiagonal entries. Using (9), the Schur parameters and complementary Schur parameters of Q_+ are related to the Givens rotation parameters through

$$|\gamma_k| = |c_k|, \qquad \sigma_k = s_k, \quad k = 1, \ldots, n-1. \tag{12}$$

Moreover, it follows easily from the minimization property (1) of GMRES that, with $\|b\| = 1$,

$$\|r_k\| = \prod_{j=1}^{k} |s_j\,|, \qquad k = 1, \ldots, n-1, \tag{13}$$

see, e.g., [2, Section 6.5.5, p. 166]. This results in the next theorem.

Theorem 7. *Consider GMRES applied to (A, b) with corresponding residual norms $\|r_0\|, \|r_1\|, \ldots, \|r_{n-1}\|$. The following assertions are equivalent:*

1- (B, c) is GMRES(A, b)-equivalent and B is unitary.

2- *The Arnoldi process applied to (B, c) generates the decomposition $BX = XQ_+$ where X is unitary, Q_+ is a unitary upper Hessenberg matrix with positive subdiagonal entries and the Schur parameters of Q_+ satisfy*

$$|\gamma_k| = \|r_k\| \sqrt{\frac{1}{\|r_k\|^2} - \frac{1}{\|r_{k-1}\|^2}}, \qquad k = 1, \ldots, n-1.$$

PROOF. For the first implication, note that Q_+ has positive subdiagonal entries because it is the Hessenberg matrix resulting from the Arnoldi process, with X denoting the unitary matrix of the associated Arnoldi vectors. Because B is unitary by assumption, $Q_+ = X^* B X$ must be unitary, too. Also note that Q_+ is the Q factor of its own QR decomposition computed with Givens rotations that have real positive off-diagonal entries. Hence the Schur parameters γ_k and complementary Schur parameters σ_k, $k = 1, \ldots, n-1$ of Q_+ satisfy (12). Because (B, c) is GMRES (A, b)-equivalent, we have

$$\prod_{j=1}^{k} \sigma_j = \|r_k\|, \qquad k = 1, \ldots, n-1,$$

see (13). A straightforward argument using induction then gives

$$\sigma_k = \frac{\|r_k\|}{\|r_{k-1}\|}, \; k = 2, \ldots, n-1.$$

Using $\sigma_k = \sqrt{1 - |\gamma_k|^2}$ we have

$$|\gamma_k| = \|r_k\| \sqrt{\frac{1}{\|r_k\|^2} - \frac{1}{\|r_{k-1}\|^2}}.$$

For the opposite implication, first note that B is unitary because so are Q_+ and X. It follows from $|\gamma_k| = \|r_k\| \sqrt{\frac{1}{\|r_k\|^2} - \frac{1}{\|r_{k-1}\|^2}}$ and from $\sigma_k = \sqrt{1 - |\gamma_k|^2}$ that the complementary Schur parameters of Q_+ are

$$\sigma_k = \frac{\|r_k\|}{\|r_{k-1}\|}, \; k = 2, \ldots, n-1.$$

They are identical with the Givens sines because Q_+ is the Q factor of its own QR decomposition. Then, because of (13), the kth GMRES residual norm ρ_k generated by (B, c) is

$$\rho_k = \prod_{j=1}^{k} s_j = \prod_{j=1}^{k} \sigma_j = \|r_k\|, \qquad k = 1, \ldots, n-1. \qquad \square$$

We remark that with Theorem 7 we can write the entries of Q_+ as a function of the residual norms. Consider the column k of the matrix Q_+. Denoting $\gamma_k = |\gamma_k| e^{\mathbf{i}\phi_k}$, the entry in the first row is

$$q_{1,k} = -\sigma_1 \cdots \sigma_{k-1}\gamma_k = -e^{\mathbf{i}\phi_k}\left(\|r_{k-1}\|^2 - \|r_k\|^2\right)^{1/2}. \tag{14}$$

The entry in row $j \le k$ is

$$\begin{aligned} q_{j,k} &= -\gamma_{j-1}\sigma_j \cdots \sigma_{k-1}\gamma_k \\ &= -e^{\mathbf{i}(\phi_{j-1}+\phi_k)}\left(\frac{1}{\|r_{j-1}\|^2} - \frac{1}{\|r_{j-2}\|^2}\right)^{1/2}\left(\|r_{k-1}\|^2 - \|r_k\|^2\right)^{1/2}, \end{aligned}$$

where we use the convention $\sigma_k \cdots \sigma_{k-1} \equiv 1$. Finally, as we already know, $q_{k+1,k} = \sigma_k = \|r_k\|/\|r_{k-1}\|$.

The previous theorem shows that for the upper Hessenberg matrix generated by the Arnoldi process applied to a unitary GMRES (A, b)-equivalent pair, its Schur parameters give the residual norms and, except for the phase angles, the residual norms determine the Schur parameters.

Note that the upper Hessenberg matrix analyzed in [11] is the specific matrix where all Schur parameters are chosen to be real positive. The upper Hessenberg matrix Q^+ in (5) does not have a positive subdiagonal, but the entries of its first row satisfy

$$q^+_{1,k} = \eta_k \equiv \sqrt{\|r_{k-1}\|^2 - \|r_k\|^2}, \quad k = 1, \ldots, n-1, \quad q^+_{1,n} = \eta_n \equiv \|r_{n-1}\|,$$

see [13, Theorem 3.4], and they have the same moduli as in (14). Here η_k represents the progress GMRES makes at the iteration step k; see [4, 5, 6].

Theorem 7 leads to the following characterization.

Corollary 8. *The following assertions are equivalent:*

1- (B, c) is GMRES(A, b)-equivalent and B is unitary,

2- The matrix B and the vector c are of the form

$$B = XV^*WX^*, \qquad c = Xe_1,$$

where X is any unitary matrix, V is a unitary matrix whose first k columns give a basis of $\mathcal{K}_k(A, b)$ for $1 \le k \le n$ and W is a unitary matrix whose first k columns give a basis of $A\mathcal{K}_k(A, b)$ for $1 \le k \le n$.

Proof. With Theorem 7, (B,c) is GMRES(A,b)-equivalent and B is unitary if and only if the matrix B and the vector c are of the form

$$B = XQ_+X^*, \qquad c = Xe_1,$$

where X is unitary and Q_+ is a unitary upper Hessenberg matrix with real positive subdiagonal whose Schur parameters satisfy

$$|\gamma_k| = \|r_k\|\sqrt{\frac{1}{\|r_k\|^2} - \frac{1}{\|r_{k-1}\|^2}}, \quad k = 1, \ldots, n-1, \qquad |\gamma_n| = 1.$$

It is easy to see that all unitary Hessenberg matrices generated by unitary GMRES(A,b)-equivalent pairs are diagonal unitary row and column scalings of each other. For example, denoting $\gamma_k = |\gamma_k|e^{\mathbf{i}\phi_k}$, Q_+ is a diagonal unitary row and column scaling

$$Q_+ = D_5^* Q_{++} D_6, \quad D_5^* = \mathrm{diag}(1, e^{-\mathbf{i}\phi_1}, \ldots, e^{-\mathbf{i}\phi_{n-1}}),\ D_6 = \mathrm{diag}(e^{\mathbf{i}\phi_1}, \ldots, e^{\mathbf{i}\phi_n}) \tag{15}$$

of the upper Hessenberg matrix Q_{++} where all Schur parameters are real positive.

A particular unitary GMRES(A,b)-equivalent pair is (S,e_1) with $S = \hat{V}^*\hat{W}$ where $\hat{V}$ is a unitary matrix whose first k columns give a basis of $\mathcal{K}_k(A,b)$ and $\hat{W}$ is a unitary matrix whose first k columns give a basis of $A\mathcal{K}_k(A,b)$ for $1 \le k \le n$, see (8). Note that because of Lemma 3, S is a unitary row and column scaling of Q^+ in that lemma and is, in particular, upper Hessenberg. Therefore the Arnoldi process for the pair (S,e_1) generates a unitary upper Hessenberg matrix which is a diagonal unitary scaling of $\hat{V}^*\hat{W}$ and the upper Hessenberg matrix Q_+ generated by *any* unitary GMRES(A,b)-equivalent pair can be written as $Q_+ = D_7^* S D_8 = (\hat{V}D_7)^*\hat{W}D_8$ for appropriate diagonal unitary matrices D_7 and D_8. □

We see that like unitary GMRES(A,b)-equivalent *matrices* (see Theorem 5), unitary GMRES(A,b)-equivalent *pairs* are determined (here up to unitary equivalence expressed by X in Corollary 8), by orthonormal bases for the Krylov subspaces $\mathcal{K}_k(A,b)$ and Krylov residual subspaces $A\mathcal{K}_k(A,b)$ for $1 \le k \le n$.

2.3. Unitary spectra and convergence behavior of GMRES

It is clear from the previous sections that there exist unitary GMRES (A, b)-equivalent matrices with different spectra: With Proposition 2 the same convergence curve can be generated with the spectrum of $W\mathcal{Q}W^*$ and with the spectrum of $WD_1\mathcal{Q}W^*$ where D_1 represents any diagonal unitary scaling. Similarly, there exist unitary system matrices of GMRES (A, b)-equivalent pairs with different spectra. This follows for instance from Theorem 7, where the same convergence curve is generated for all choices of phase angles of the involved Schur parameters. We can also prove the following result.

Proposition 9. *Consider GMRES applied to an unreduced unitary Hessenberg matrix Q with the right-hand side e_1 and zero initial guess. The following assertions are equivalent:*

1- $\tilde{Q}$ is unitary and GMRES (Q, e_1)-equivalent,

2- $\tilde{Q} = D_1 Q D_2$, where D_i, $i = 1, 2$ are diagonal unitary matrices.

Proof. For all $k \leq n$, an orthogonal basis for $\mathcal{K}_k(Q, e_1)$ is given by the unit vectors $e_1, \ldots, e_k$ and an orthogonal basis for

$$Q\mathcal{K}_k(Q, e_1) = \text{span}\{Qe_1, Q^2e_1, \ldots, Q^ke_1\}$$

is given by the first k columns of Q. Therefore, with Theorem 5, $\tilde{Q} = WV^*$ where W is a diagonal unitary column scaling of Q and V is a diagonal unitary column scaling of the identity matrix I. □

In the following numerical experiments we take $n = 50$ and for given eigenvalues on the unit circle and an initial vector, we generate the unitary upper Hessenberg matrix Q_+ with real positive subdiagonal by applying the Arnoldi process to the corresponding diagonal matrix Λ, i.e., $\Lambda X = XQ_+$. The spectrum is chosen to have two clusters within the semi-angle 10 and 5 degrees around 1 and -1 respectively, each containing 20 eigenvalues. The other 10 eigenvalues are distributed uniformly within the remaining parts of the unit circle; see the left part of Figure 1. The initial Arnoldi vector is chosen to have all its entries equal, i.e., from $Q_+ = X^*\Lambda X$ it implies that the first column of X, which is equal to the first row of the eigenvector matrix X^* has all its entries equal to $1/\sqrt{n}$. Applying GMRES to (Q_+, e_1)

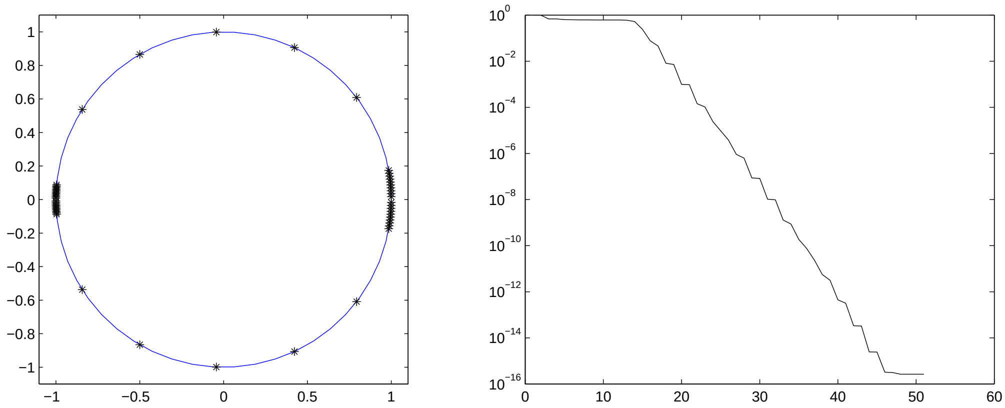

Figure 1: Spectrum (left) of the matrix Q_+ and the GMRES residual norms for the pair (Q_+, e_1).

gives the residual norms shown in the right part of Figure 1. The first 12 Schur parameters of Q_+ (see (11) and Theorem 7) are of small size and the remaining ones have absolute value close to one.

Now we change the phase angles of the Schur parameters of Q_+ to make them real and positive. This gives the unitary upper Hessenberg matrix Q_{++}; see (15) and [11]. Obviously, applying GMRES to (Q_{++}, e_1) gives the same residual norms as before. The eigenvalues and the size of the squared first entries of the eigenvectors are for Q_{++}, however, different from those of Q_+. They are plotted in Figure 2, where the eigenvectors are ordered increasingly with respect to the phase angle of the corresponding eigenvalues (with the smallest phase angle being $-\pi$ and the largest being π).

We can generate yet another GMRES$\,(Q_+, e_1)$-equivalent pair by using Proposition 9. For instance let $\tilde{Q} = D_1 Q_+ D_2$ with

$$D_1 = \mathrm{diag}\,(e^{2\pi\mathbf{i}/50}, e^{4\pi\mathbf{i}/50}, e^{6\pi\mathbf{i}/50}, \ldots, e^{2\pi\mathbf{i}}), \qquad D_2 = I.$$

Figure 3 plots for $\tilde{Q}$ the information analogous to Figure 2. The spectrum of $\tilde{Q}$ and the first components of its eigenvectors are clearly different from that of both Q_+ and Q_{++}.

Summarizing, there is no characteristic unitary spectrum corresponding to a certain GMRES convergence curve; many unitary spectra can be in general associated with the same curve. On the other hand, the bound (2) for a unitary GMRES$\,(A, b)$-equivalent pair with $\kappa(Z) = 1$ seemingly

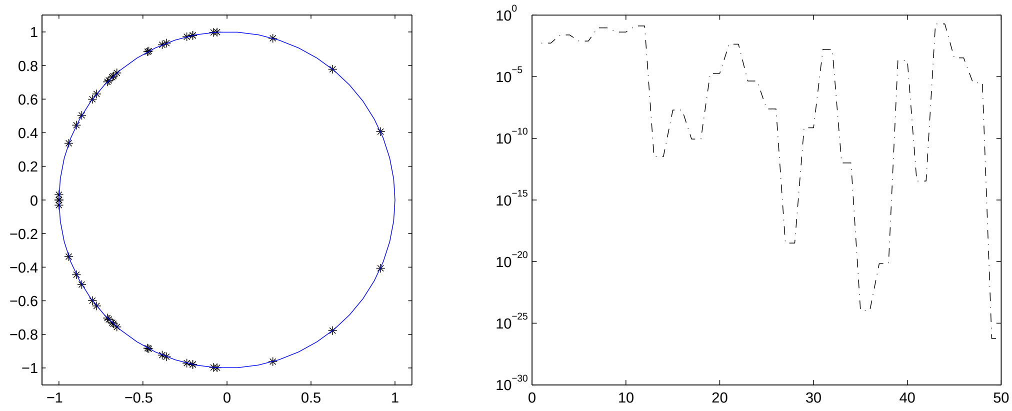

Figure 2: Eigenvalues (left) and size of the squared first components of the associated eigenvectors of the matrix Q_{++}. The eigenvectors are in increasing order with respect to the phase angle of the eigenvalues.

suggests a relation between a unitary spectrum and GMRES convergence. Such interpretation of (2) is, however, misleading. One must be careful with linking the bound (2) to GMRES convergence, even if the matrix is normal. We remark that when the matrix A is Hermitian with real distinct eigenvalues, the right-hand side of (2) takes the value

$$\min_{p\in\Pi_k}\max_{i=1,\dots,n}|p_k(\lambda_i)| = \left(\sum_{j=1}^{k+1}\Pi_{i=1,i\neq j}^{k+1}\frac{|\mu_i|}{|\mu_i-\mu_j|}\right)^{-1} \tag{16}$$

for a subset $\{\mu_1,\dots,\mu_{k+1}\}$ of $k+1$ eigenvalues of $\{\lambda_1,\dots,\lambda_n\}$, see [22]. However, as soon as one eigenvalue of A is complex, equation (16) does not hold in general [23]. We have the following facts for a unitary A.

If the spectrum of a unitary matrix has a large maximum gap, then we have fast GMRES convergence. This was shown in [9]. On the other hand, *if* we have fast GMRES convergence, then there does not need to be a large gap in the spectrum of the unitary matrix A; the fast convergence can be assured by a particular decomposition of b in the invariant subspaces of A. If Q_+ is the corresponding upper Hessenberg matrix resulting from the Arnoldi process applied to (A,b), then (Q_+,e_1) is a unitary GMRES (A,b)-equivalent pair where Q_+ has the same spectrum as the unitary matrix A. Since the right-hand side e_1 for the pair (Q_+,e_1) is independent of A and b, the interplay of A and b has been in some sense wrapped into the entries of Q_+. Of

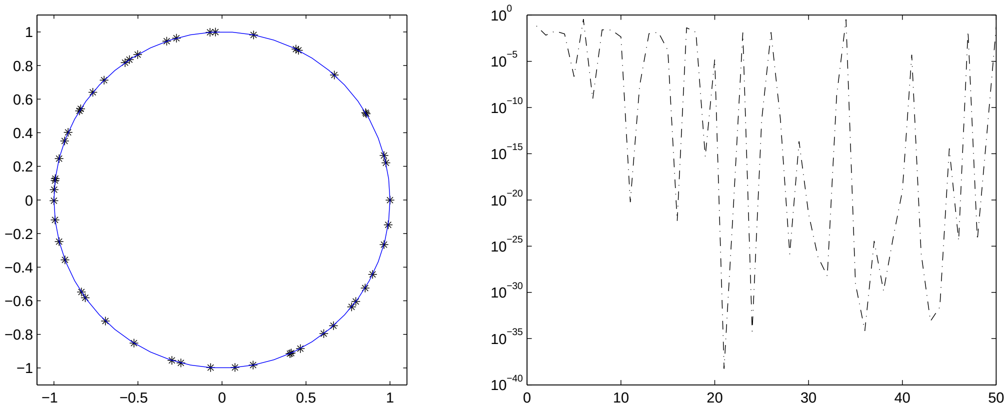

Figure 3: Spectrum (left) and size of the squared first components of the associated eigenvectors of the matrix $\tilde{Q}$. The eigenvectors are in increasing order with respect to the phase angle of the eigenvalues.

course, convergence still depends on how rich e_1 is in the various eigenvectors of Q_+. However, if we scale Q_+ with unitary diagonal matrices D_1 and D_2 such that $Q_{++} = D_1 Q_+ D_2$ has only real positive Schur parameters, then, according to [11], fast convergence corresponds to a large gap in the spectrum of the Hessenberg matrix Q_{++}. The pair (Q_{++}, e_1) is another unitary GMRES (A, b)-equivalent pair (by Proposition 9). This pair does not result from the Arnoldi process for (A, b). It results from the Arnoldi process for a pair $(\tilde{A}, \tilde{b})$ where the eigenvalues of the unitary matrix $\tilde{A}$ must contain the same large gap as the spectrum of Q_{++}. GMRES applied to this matrix $\tilde{A}$ with an arbitrary right-hand side will exhibit fast convergence, see [9].

If we have stagnation of GMRES, then all corresponding unitary spectra have a very regular structure. This is shown in the following result first proved in [24]; here we give a shorter proof.

Proposition 10. *Let the GMRES method for a pair (A, b) where A has order n stagnate until the last iteration. The following assertions are equivalent:*

1- *There exists a vector c such that (B, c) is a GMRES(A, b)-equivalent pair and B is unitary,*

2- *The spectrum of the unitary matrix B is given by the roots of the equation $\lambda^n = e^{\mathbf{i}\phi}$ for a real number ϕ.*

PROOF. Let (B, c) be a GMRES (A, b)-equivalent pair. Because of Theorem 7, the Arnoldi process applied to this pair generates a unitary upper Hessenberg matrix Q_+ whose Schur parameters are all zero, except for γ_n with $|\gamma_n| = 1$, i.e. $\gamma_n = e^{\mathbf{i}\phi}$ for a real number ϕ. Then the Hessenberg matrix Q_+ is nothing but the companion matrix for the polynomial $\lambda^n - e^{\mathbf{i}\phi}$ (see (10)). The claim follows because B is obtained from Q_+ using a similarity transformation, see Theorem 7. Inversely, let the spectrum of the unitary matrix B be given by the roots of the equation $\lambda^n = e^{\mathbf{i}\phi}$ for a real number ϕ and let $B = Z_B \Lambda Z_B^*$ be the spectral decomposition of B with unitary Z_B. If C is the companion matrix for the polynomial $\lambda^n - e^{\mathbf{i}\phi}$, then it is also unitary and has the spectral decomposition $C = Z_C \Lambda Z_C^*$ with unitary Z_C. We can write B as

$$B = Z_B \Lambda Z_B^* = Z_B Z_C^* C Z_C Z_B^* = XCX^*, \quad X \equiv Z_B Z_C^*,$$

with X unitary. Thus we have $BX = XC$ and if we put $X = [x_1, \ldots, x_n]$, then

$$x_j = Bx_{j-1}, \quad j = 2, \ldots, n$$

and

$$x_j = B^{j-1} x_1, \quad j = 2, \ldots, n, \qquad Bx_n = e^{\mathbf{i}\phi} x_1.$$

This means that with the choice $c \equiv x_1$

$$B\mathcal{K}_n(B, c) = \text{span}\{x_2, \ldots, x_n, x_1\}.$$

Thus for $k < n$, $x_1 = c \perp B\mathcal{K}_k(B, c) = \text{span}\{x_2, \ldots, x_{k+1}\}$ and GMRES applied to (B, c) stagnates until the last step. □

The previous proposition shows that complete stagnation is possible for GMRES with a unitary matrix B only if the spectrum of B represents a rotation of the roots of unity. But *if* the spectrum of a unitary matrix B represents a rotation of the roots of unity, this needs not imply complete stagnation of GMRES applied to B with an arbitrary right-hand side. It holds for some specific choice of c.

In a more general context it is worth mentioning the paper [25] where the isometric Arnoldi process is analyzed asymptotically using potential theory. In particular, the paper defines and investigates the isometric Arnoldi minimization problem and makes analogies between the properties of unitary Hessenberg matrices with positive diagonals and Jacobi matrices.

In the next section we derive an expression for the residual norms in terms of eigenvalues *and* eigenvector components when GMRES is applied to a normal matrix.

3. GMRES residual norms for normal matrices

Let the Arnoldi process applied to the pair (A, b) with normal A generate the unreduced Hessenberg matrix H_+ and the unitary matrix $\hat{V}$ satisfying (4). Since $\hat{V}^* b = e_1$, GMRES generates with (A, b) the same residual norms as with (H_+, e_1). We will therefore consider the pairs (H_+, e_1) with normal unreduced upper Hessenberg matrices. First we need the following lemma, which also holds for non-normal H_+.

Lemma 11. *Let H_+ be an unreduced Hessenberg matrix with real positive subdiagonal, C be the companion matrix corresponding to its characteristic polynomial and let*

$$U = \left[\begin{array}{cccc} e_1 & H_+ e_1 & \cdots & H_+^{n-1} e_1 \end{array}\right], \tag{17}$$

which is an upper triangular matrix with real positive diagonal entries. Then

$$H_+ = UCU^{-1}.$$

PROOF. See [26, Lemma 2] and [27, Equation (2.4)]. □

The matrix H_+ is a *normal* unreduced upper Hessenberg matrix with real positive subdiagonal if and only if U in (17) is the Cholesky factor of a moment matrix. This is stated more precisely in the next result, which is due to Parlett [28]. Note that an unreduced normal Hessenberg matrix is diagonalizable and it has distinct eigenvalues.

Theorem 12. *Let H_+ be an unreduced Hessenberg matrix having real positive subdiagonal entries. Let all its eigenvalues λ_i, $i = 1, \ldots, n$ be distinct and let U be the upper triangular matrix in (17). Then the following statements are equivalent:*

1- H_+ is normal.

2- *There exist real positive weights* ω_k *with* $\sum_{k=1}^{n} \omega_k = 1$ *such that* $M = U^*U$ *is the moment matrix with entries defined by*

$$M_{i,j} = \sum_{k=1}^{n} \omega_k (\bar{\lambda}_k)^{i-1} \lambda_k^{j-1}. \tag{18}$$

Proof. See [28]. □

For the proof see also [27, p. 392].

The weights in the second assertion are the squares of the moduli of the first components of the eigenvectors of H_+. Indeed, with the spectral factorization $H_+ = Z\text{diag}\,(\lambda_1, \ldots, \lambda_n)Z^* = Z\Lambda Z^*$ we get

$$U = Z \begin{bmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{bmatrix}, \qquad c = Z^* e_1,$$

which gives

$$M = U^*U = \begin{bmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{bmatrix}^* \begin{bmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{bmatrix}.$$

Comparing with (18) we obtain $\omega_k = |\, e_k^T c|^{\,2}$.

The residual norms generated by GMRES can be expressed in terms of the moment matrix $M = U^*U$ as follows. Let

$$K = [b, Ab, \ldots, A^{n-1}b]$$

be the Krylov matrix for a pair (A, b). Using (4),

$$\begin{aligned} M &= U^*U = (\hat{V}U)^*\hat{V}U \\ &= \left(\hat{V} \begin{bmatrix} e_1 & H_+e_1 & \cdots & H_+^{n-1}e_1 \end{bmatrix}\right)^* \hat{V} \begin{bmatrix} e_1 & H_+e_1 & \cdots & H_+^{n-1}e_1 \end{bmatrix} \\ &= \left(\begin{bmatrix} b & Ab & \cdots & A^{n-1}b \end{bmatrix}\right)^* \begin{bmatrix} b & Ab & \cdots & A^{n-1}b \end{bmatrix} = K^*K. \end{aligned}$$

It has been proved in several publications (see, e.g., [29, Theorem 4.1] and [30, Lemma 1]), that if M_k denotes the kth leading principal submatrix of $M = K^*K$, then the kth GMRES residual norm $\|r_k\|$ satisfies

$$\|r_k\|^2 = \frac{1}{(M_{k+1}^{-1})_{1,1}}. \tag{19}$$

In [31, Theorem 2.1] the same result is written slightly differently and it is pointed out that the formula goes back to [32, Section 3 and 4], see also [33, Theorem 2.1] and the remarks thereafter. Note that the formula (19) holds for general, not necessarily normal A. In the normal case it leads to the main result of this section.

Theorem 13. *Let A be a normal matrix with distinct eigenvalues and the spectral factorization $Z\Lambda Z^*$ where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$, $Z^*Z = ZZ^* = I$. Let b be a vector of unit norm such that all entries of the vector $c \equiv Z^*b$ are nonzero and let $\sum_{I_k}$ denote summation over all possible sets I_k of k indices $i_1, i_2, \ldots, i_k$ such that $1 \leq i_1 < \cdots < i_k \leq n$. The residual norms of GMRES applied to (A, b) then satisfy*

$$\|r_1\|^2 = \frac{\sum_{I_2} \omega_{i_1}\omega_{i_2} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_2 \\ i_\ell, i_j \in I_2}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{i=1}^{n} \omega_i |\lambda_i|^2}, \tag{20}$$

and for $k = 2, \ldots, n-1$,

$$\|r_k\|^2 = \frac{\sum_{I_{k+1}} \left[\prod_{j=1}^{k+1} \omega_{i_j}\right] \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{I_k} \left[\prod_{j=1}^{k} \omega_{i_j} |\lambda_{i_j}|^2\right] \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_k \\ i_\ell, i_j \in I_k}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}, \tag{21}$$

where $\omega_{i_j} = |e_{i_j}^T c|^2$.

Proof. Using (19) and Cramer's rule:

$$\|r_k\|^2 = \frac{1}{(M_{k+1}^{-1})_{1,1}} = \frac{\det(M_{k+1})}{\det(M_{2:k+1,2:k+1})},$$

where $M_{2:k+1,2:k+1}$ is the $k \times k$ trailing principal submatrix of M_{k+1}. We can write M_{k+1} as

$$M_{k+1} = \mathcal{V}_{k+1}^* D_\omega \mathcal{V}_{k+1} = (\mathcal{V}_{k+1}^* D_\omega^{1/2})(D_\omega^{1/2}\mathcal{V}_{k+1}) \equiv F^*F, \tag{22}$$

where

$$\mathcal{V}_{k+1} = \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^k \\ 1 & \lambda_2 & \cdots & \lambda_2^k \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_n & \cdots & \lambda_n^k \end{pmatrix},$$

is an $n \times (k+1)$ Vandermonde matrix and D_ω a diagonal matrix of order n with $\omega_1, \ldots, \omega_n$ on the diagonal. Similarly,

$$M_{2:k+1,2:k+1} = \mathcal{V}_k^* \Lambda^* D_\omega \Lambda \mathcal{V}_k = (\mathcal{V}_k^* D_\omega^{1/2} \Lambda^*)(\Lambda D_\omega^{1/2} \mathcal{V}_k) \equiv G^*G.$$

Let us first consider the determinant of M_{k+1}. Let $F_{I_{k+1},:}$ be the square submatrix of F whose row indices belong to an index set I_{k+1}. Following [34], we can use the Cauchy-Binet formula[1] for the determinant of the square product of two conforming rectangular matrices. When the rectangular matrices are Hermitian transposes of each other, the formula yields

$$\det(M_{k+1}) = \sum_{I_{k+1}} |\det(F_{I_{k+1},:})|^2.$$

Thus

$$\det(M_{k+1}) = \sum_{I_{k+1}} \left[\prod_{j=1}^{k+1} \omega_{i_j}\right] |\det(\mathcal{V}_{I_{k+1}})|^2,$$

where (see [35])

$$\mathcal{V}_{I_{k+1}} = \begin{pmatrix} 1 & \lambda_{i_1} & \cdots & \lambda_{i_1}^k \\ 1 & \lambda_{i_2} & \cdots & \lambda_{i_2}^k \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_{i_{k+1}} & \cdots & \lambda_{i_{k+1}}^k \end{pmatrix}, \quad \det(\mathcal{V}_{I_{k+1}}) = \prod_{\substack{i_1 \le i_\ell < i_j \le i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} (\lambda_{i_j} - \lambda_{i_\ell}).$$

Analogously,

$$\begin{aligned} \det(M_{2:k+1,2:k+1}) &= \sum_{I_k} |\det(G_{I_k,:})|^2 \\ &= \sum_{I_k} \left[\prod_{j=1}^{k} \omega_{i_j} |\lambda_{i_j}|^2\right] |\det(\mathcal{V}_{I_k})|^2. \end{aligned}$$

Noting that for $k = 1$, the matrix $\mathcal{V}_{I_k}$ reduces to the number one, we have

$$\sum_{I_1} \left[\prod_{j=1}^{1} \omega_{i_j} |\lambda_{i_j}|^2\right] |\det(\mathcal{V}_{I_1})|^2 = \sum_{i=1}^{n} \omega_i |\lambda_i|^2 |\det(1)|^2,$$

which finishes the proof. □

[1] This formula was first proved in 1812 independently by Augustin-Louis Cauchy (1789-1857) and Jacques Binet (1786-1856).

Assuming that GMRES applied to a normal matrix A and a given right-hand side vector b does not terminate until the last step n, this theorem gives the GMRES residual norms in terms of the eigenvalues and the squared size of the components of the right-hand side vector in the direction of the individual eigenvectors. Thus Theorem 13 gives the solution of the polynomial approximation problem (3).

It can easily be extended to the case where GMRES terminates before the step n. If A has $m < n$ distinct eigenvalues and b has nonzero components in all m associated invariant subspaces, then GMRES terminates with $r_m = 0$, (20) holds and if $m > 2$, (21) holds for $k = 2, \ldots, m-1$. If b has nonzero components only in $\ell < m$ invariant subspaces corresponding to distinct eigenvalues, then GMRES terminates with $r_\ell = 0$, (20) holds and if $\ell > 2$, (21) holds for $k = 2, \ldots, \ell - 1$.

It should be pointed out that Ipsen gave in [31, Theorem 4.1] another expression for $\|r_k\|$ using a minimization problem over $k+1$ eigenvalues. In [23, Theorem 2.1], the formula (21) was derived for $k = n-1$. Formulas (20) and (21) might be of use in situations where the influence of the right-hand side is of interest. For instance, restarting in GMRES corresponds to changes in the weights ω_{i_j}. Worst case behavior corresponds to taking the maximum over the values of ω_{i_j}. Theorem 13 also leads to a straightforward lower and upper bound where the influence of b is separated from the influence of the spectrum.

Corollary 14. *With the notation of Theorem 13, let*

$$\omega_- = \min_{1 \le i \le n} \omega_i, \qquad \omega_+ = \max_{1 \le i \le n} \omega_i.$$

Then the residual norms of GMRES applied to (A, b) *satisfy*

$$\frac{\sum_{I_2} \prod_{\substack{i_1 \le i_\ell < i_j \le i_2 \\ i_\ell, i_j \in I_2}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{i=1}^n |\lambda_i|^2} \omega_- \le \|r_1\|^2 \le \frac{\sum_{I_2} \prod_{\substack{i_1 \le i_\ell < i_j \le i_2 \\ i_\ell, i_j \in I_2}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{i=1}^n |\lambda_i|^2} \omega_+ \,, \tag{23}$$

and for $k = 2, \ldots, n-1$,

$$\|r_k\|^2 \;\ge\; \frac{\sum_{I_{k+1}} \prod_{\substack{i_1 \le i_\ell < i_j \le i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{I_k} \left[\prod_{j=1}^k |\lambda_{i_j}|^2\right] \prod_{\substack{i_1 \le i_\ell < i_j \le i_k \\ i_\ell, i_j \in I_k}} |\lambda_{i_j} - \lambda_{i_\ell}|^2} \omega_-, \tag{24}$$

$$\|r_k\|^2 \;\leq\; \frac{\sum_{I_{k+1}} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{I_k} \left[\prod_{j=1}^{k} |\lambda_{i_j}|^2\right] \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_k \\ i_\ell, i_j \in I_k}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}\, \omega_+ \,. \tag{25}$$

Proof. If C and D are two matrices of sizes $n \times (k+1)$ and $n \times n$ respectively, $k \leq n-1$, and C is of full rank, then

$$\frac{\sigma_{min}(D)^2}{e_1^T (C^* C)^{-1} e_1} \leq \frac{1}{e_1^T (C^* (D^* D) C)^{-1} e_1} \leq \frac{\sigma_{max}(D)^2}{e_1^T (C^* C)^{-1} e_1}, \tag{26}$$

see [36, Lemma 1]. If we put, using the notation of the proof of Theorem 13, $C \equiv \mathcal{V}_{k+1}$ and $D \equiv D_\omega^{1/2}$, then the claim follows using exactly the same arguments as in the proof of Theorem 13. □

The bounds are attained for $\omega_- = \omega_+$, that is, for all components of the right hand side in the eigenvector basis of the same size. In that case the bounds are attained for all k, i.e. one choice of b guarantees the equality throughout the entire GMRES process. In comparison, the standard bound (2) with $\kappa(Z) = 1$ is fully dependent on eigenvalues, but it is attained at iteration k for a specific right-hand side which depends upon k. Moreover, (2) is an upper bound only; Corollary 14 gives both lower and upper bounds showing the descriptive role of eigenvalues for the behaviour of GMRES in the normal case.

When A is unitary, the eigenvalues are of modulus one and (20) and (21) simplify to

$$\|r_1\|^2 = \sum_{I_2} \omega_{i_1} \omega_{i_2} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_2 \\ i_\ell, i_j \in I_2}} |\lambda_{i_j} - \lambda_{i_\ell}|^2$$

and

$$\|r_k\|^2 = \frac{\sum_{I_{k+1}} \prod_{j=1}^{k+1} \omega_{i_j} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}{\sum_{I_k} \prod_{j=1}^{k} \omega_{i_j} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_k \\ i_\ell, i_j \in I_k}} |\lambda_{i_j} - \lambda_{i_\ell}|^2}, \tag{27}$$

respectively. We see that the GMRES convergence for unitary matrices depends strongly on the angles between pairs of eigenvalues on the unit circle. As it is obvious, the residual norms stay the same when all eigenvalues are rotated by a given angle (without modifying the eigenvectors).

Formula (27) for the GMRES residual norm, which holds at every iteration step, offers an insight to the fact that outlying eigenvalues can often be associated with an initial stage of slow GMRES convergence (see, e.g., [37] where the emphasis is on the asymptotic convergence factor after the initial stage). From (27) we see that if there is one tight cluster of eigenvalues and, say, m other eigenvalues well separated from this cluster, then after $m+1$ iterations there will be at least one small factor $|\lambda_{i_j} - \lambda_{i_\ell}|^2$ in every summation term of the numerator because $m+2$ eigenvalues are involved and at least one pair of eigenvalues will belong to the cluster. If the weights are of similar size, one can therefore expect acceleration of convergence after the m initial steps.

An analogous argument can be used in the presence of multiple clusters; with ℓ well separated clusters and another m well separated single eigenvalues, acceleration might be expected after $m+\ell$ steps. This offers an explanation for the acceleration of convergence after 13 steps in Figure 1, Section 2.3, where the spectrum was chosen to have two clusters, the other 10 eigenvalues were regularly distributed around the remaining portions of the unit circle and all weights were chosen to be equal. Here the sharpness of the start of the acceleration as well as the approximate slope of the convergence curve for $k > 13$ depend on the tightness of the clusters in comparison with the mutual distance of the well-separated eigenvalues. A bad configuration is when the eigenvalues are almost regularly distributed on the unit circle and the weights are all of similar size.

Corollary 8 and (27) finally give the following statement.

Theorem 15. *Let V be a unitary matrix whose first k columns give a basis of the Krylov space $\mathcal{K}_k(A,b)$ and W be a unitary matrix whose first k columns give a basis of the Krylov residual space $A\mathcal{K}_k(A,b)$ for $1 \leq k \leq n$. Using the notation of Theorem 13, the residual norms of GMRES applied to (A,b) satisfy*

$$\|r_1\|^2 = \sum_{I_2} \omega_{i_1}\omega_{i_2} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_2 \\ i_\ell, i_j \in I_2}} |\,\delta_{i_j} - \delta_{i_\ell}|^2\,,$$

$$\|r_k\|^2 = \frac{\sum_{I_{k+1}} \prod_{j=1}^{k+1} \omega_{i_j} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_{k+1} \\ i_\ell, i_j \in I_{k+1}}} |\delta_{i_j} - \delta_{i_\ell}|^2}{\sum_{I_k} \prod_{j=1}^{k} \omega_{i_j} \prod_{\substack{i_1 \leq i_\ell < i_j \leq i_k \\ i_\ell, i_j \in I_k}} |\delta_{i_j} - \delta_{i_\ell}|^2}, \quad k = 2, \ldots, n,$$

where the δ_i *are the eigenvalues in the generalized eigenvalue problem*

$$Wx = \delta V x$$

and the ω_i *are the squared moduli of the first components of the corresponding eigenvectors.*

4. Conclusion

We investigate GMRES (A, b)-equivalent pairs (B, c), where B is unitary. We characterize B in terms of orthonormal bases for the sequence of Krylov subspaces $\mathcal{K}_k(A, b)$ and Krylov residual subspaces $A\mathcal{K}_k(A, b)$, $k = 1, 2, \ldots, n$. This shows that a possible linking of the spectral properties of unitary GMRES (A, b)-equivalent matrices, which influence GMRES convergence behavior, to some simple properties of A would be, in general, rather difficult. We also offer some insight concerning the substantial role of the right-hand side vector components in the direction of the individual eigenvectors. The presented formula giving the residual norms for normal matrices can for some particular eigenvalue distribution explain acceleration of convergence of GMRES observed after a number of iterations.

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