ANY ADMISSIBLE HARMONIC RITZ VALUE SET IS POSSIBLE FOR PRESCRIBED GMRES RESIDUAL NORMS

KUI DU

Abstract. We show that any admissible harmonic Ritz value set is possible for prescribed GMRES residual norms, which is a complement for the results in [Duintjer Tebbens and Meurant, SIAM J. Matrix Anal. Appl., 33 (2012), no. 3, pp. 958–978].

Key words. Harmonic Ritz values, GMRES, prescribed residual norms

AMS subject classifications. 65F10, 65F15, 65F18

1. Introduction. The generalized minimal residual method (GMRES) [10] is a popular iterative technique for solving large non-Hermitian linear systems. Greenbaum and Strakoš [6] proved that any convergence curve for the residual norm can be generated by GMRES applied to a non-derogatory matrix having prescribed eigenvalues. Greenbaum, Pták, and Strakoš [5] showed later that any nonincreasing convergence curve is possible for GMRES. Arioli, Pták, and Strakoš [1] gave a complete parametrization for the class of matrices having the same GMRES convergence curve.

Recently, Duintjer Tebbens and Meurant [3] showed that any Ritz value behavior is possible for prescribed GMRES residual norms. Since the roots of the polynomials GMRES generates to compute its residuals are harmonic Ritz values [4], it is interesting to investigate the harmonic Ritz value behavior for prescribed GMRES residual norms. Duintjer Tebbens and Meurant wrote [3, page 974] it is not clear whether any harmonic Ritz value behavior is possible for prescribed GMRES residual norms. In this note we show that any admissible harmonic Ritz value set (introduced in §3) is possible for prescribed GMRES residual norms.

The rest of this note is organized as follows. In the remainder of this section we introduce some notations. In section 2 we give some properties for GMRES and harmonic Ritz values. In section 3 we provide the main result of this note by exploiting a parameterized inverse eigenvalue problem.

To facilitate the discussion, we shall adopt the following notations. For a matrix $A$, let $a_{ij}$, $a_k$, $\text{tr}(A)$, $\det(A)$, $A_k$, $\tilde{A}_k$ and $A^*$ denote the $i,j$ entry, the $k$th column, the trace, the determinant, the $k \times k$ principal submatrix, the matrix build with the first $k$ columns, and the conjugate transpose of $A$, respectively. The complex conjugate of a scalar $z$ is written $\overline{z}$. Let $e_k$ denote the $k$th column of the identity matrix of appropriate order.

2. Preliminaries. Let a nonsingular matrix $A \in \mathbb{C}^{n \times n}$ and a vector $b \in \mathbb{C}^n$ be given. For an initial guess $x_0$, GMRES approximates the exact solution of $Ax = b$ at step $k$ by the vector $x_k \in x_0 + K_k(A, r_0)$ that minimizes the Euclidean norm of the residual $r_k := b - Ax_k$, i.e.,

$$\|r_k\| = \min_{x \in x_0 + K_k(A, r_0)} \|b - Ax\|,$$

*School of Mathematical Sciences and Fujian Provincial Key Laboratory of Mathematical Modelling and High-Performance Scientific Computation, Xiamen University, Xiamen 361005, China (kuidu@xmu.edu.cn). The research of this author was supported by the National Natural Science Foundation of China (No.11201392 and No.91430213), the Doctoral Fund of Ministry of Education of China (No.20120121120020), and the Fundamental Research Funds for the Central Universities (No.20720160002).
where

\[ K_k(A, r_0) := \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}. \]

The Arnoldi process [2] constructs an orthonormal basis of \( K_k(A, r_0) \). Without loss of generality we assume

\[ \|r_0\| = 1, \]

and we also assume that the Arnoldi process for the pair \( \{A, r_0\} \) do not break down before the \( n \)-th iteration. Then we have the Arnoldi relation

\[ \text{(2.1)} \quad AV = VH, \]

where \( V \) is unitary and \( H \) is irreducible upper Hessenberg. The columns of \( \tilde{V}_k \) form an orthonormal basis of \( K_k(A, r_0) \).

The eigenvalues of the generalized eigenvalue problem

\[ \text{(2.2)} \quad \tilde{H}_k^*\tilde{H}_k z = \theta k H_k^* z \]

are called harmonic Ritz values at step \( k \) of the Arnoldi process for \( \{A, r_0\} \), giving the \( k \)-tuple

\[ \Theta^{(k)} = (\theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_k^{(k)}). \]

For simplicity we assume these number are sorted in nondecreasing order (in magnitude). Note that \( \theta_j^{(k)} \) is either nonzero finite complex number or \( \infty \). We denote by \( \Theta \) the set

\[ \text{(2.3)} \quad \Theta := \{\Theta^{(1)}, \Theta^{(2)}, \ldots, \Theta^{(n)}\} \]

representing all \( (n + 1)n/2 \) harmonic Ritz values.

Consider a QR factorization

\[ \text{(2.4)} \quad H = QR, \]

where \( Q \) is unitary irreducible upper Hessenberg and \( R \) is nonsingular upper triangular. By \[2.3\], we have the following factorizations of \( H_k \) and \( \tilde{H}_k \):

\[ \text{(2.5)} \quad H_k = Q_k R_k, \quad \tilde{H}_k = \tilde{Q}_k R_k. \]

Entries of \( Q \) and the relation to GMRES residual norms have been shown in \[8, 9\]. For convenience of our investigation, we list some known results in Propositions \[2.1, 2.2, 2.3, 2.4\] and also give proofs for completeness.

**Proposition 2.1.** Rows 2 through \( n \) of the unitary irreducible upper Hessenberg matrix \( Q \) are uniquely determined (up to complex signs) by the first row of \( Q \). Specifically, for \( i = 1 : n - 1 \) and \( j = i + 1 : n \)

\[ q_{i+1,j} = \rho_i \frac{\sqrt{1 - \sum_{l=1}^{i} |q_{l1}|^2}}{\sqrt{1 - \sum_{l=1}^{i} |q_{l1}|^2}}, \]

\[ q_{i+1,j} = -\rho_i \frac{\sqrt{1 - \sum_{l=1}^{i} |q_{l1}|^2} \sqrt{1 - \sum_{l=1}^{i} |q_{l1}|^2}}{q_{i1} q_{ij}}. \]
where

\[ |\rho_1| = |\rho_2| = \cdots = |\rho_{n-1}| = 1. \]

The proof of Proposition 2.1 is straightforward by explicit calculations (exploiting the unitary irreducible upper Hessenberg structure of \( Q \)).

**Proposition 2.2.** GMRES residual norm at step \( k \), \( \|r_k\| \), is given by

\[
\|r_k\| = \left( \sum_{l=k+1}^{n} |q_{ll}|^2 \right)^{1/2}.
\]

**Proof.** It follows from \( \tilde{H}_k = \tilde{Q}_k R_k \) and

\[
\|r_k\| = \min_{x \in x_0 + K_k(A, r_0)} \|b - Ax\|
\]

\[
= \min_{y \in C^k} \|r_0 - A \tilde{V}_k y\|
\]

\[
= \min_{y \in C^k} \|r_0 - V \tilde{H}_k y\|
\]

\[
= \min_{y \in C^k} \|e_1 - \tilde{H}_k y\|
\]

that

\[
\|r_k\| = \|(I - \tilde{Q}_k \tilde{Q}_k^*) e_1\| = \left( \sum_{l=k+1}^{n} |q_{1l}|^2 \right)^{1/2} = \left( \sum_{l=k+1}^{n} |q_{ll}|^2 \right)^{1/2}.
\]

Proposition 2.2 implies that the GMRES residual norms can be read from the first row of \( Q \).

**Proposition 2.3.** GMRES applied to \( \{A, r_0\} \) stagnates at step \( k \), i.e.,

\[
\|r_k\| = \|r_{k-1}\|,
\]

if and only if \( q_k \), the \( k \)th column of \( Q \), satisfies

\[ q_k = q_{k+1,k} e_{k+1}. \]

**Proof.** It follows from Proposition 2.2 and \( \|r_k\| = \|r_{k-1}\| \) that \( q_{1k} = 0 \). Then \( q_{ik} = 0 \) for \( i = 2 : k \) follows from Proposition 2.1. Therefore \( q_k = q_{k+1,k} e_{k+1} \).

Conversely, if \( q_k = q_{k+1,k} e_{k+1} \), by Proposition 2.2, \( \|r_k\| = \|r_{k-1}\| \).

Next, we characterize the harmonic Ritz values when GMRES stagnates. By (2.4), the generalized eigenvalue problem (2.2) for harmonic Ritz values at step \( k \) reduces to:

\[
R_k z = \theta Q_k^* z.
\]

**Proposition 2.4.** Assume that GMRES applied to \( \{A, r_0\} \) stagnates from step \( k + 1 \) to step \( k + m \) (\( 0 \leq k < k + m \leq n - 1 \)), i.e.,

\[
\|r_k\| = \|r_{k+1}\| = \cdots = \|r_{k+m}\|.
\]
Then harmonic Ritz values \( \{ \theta_j^{(k+i)} \}_{j=1}^{k+i} \) at step \( k+i \) for \( i = 1 : m \) satisfy

\[
\begin{align*}
\theta_j^{(k+i)} &= \begin{cases} 
\theta_j^{(k)}, & 1 \leq j \leq k \\
\infty, & k+1 \leq j \leq k+i.
\end{cases}
\end{align*}
\]

**Proof.** By Proposition 2.3, the generalized eigenvalue problem (2.6) at step \( k+i \) for \( i = 1 : m \) reduces to

\[
R_{k+i}z = \theta \begin{bmatrix} Q_k^* & 0 \\ 0 & T \end{bmatrix} \begin{bmatrix} 7_{k+1,k}e_ke_1^* \\ T \end{bmatrix} z.
\]

The statement follows from \( R_{k+i} \) is nonsingular upper triangular, and all diagonal entries of the upper triangular matrix \( T \) are zero.

**3. Harmonic Ritz values for prescribed GMRES residual norms.** We call a set \( \Theta \) defined in (2.3) satisfying \( \infty \notin \Theta \) an admissible harmonic Ritz value set for stagnation-free GMRES. We also call a set \( \Theta \) defined in (2.3) satisfying Proposition 2.4 an admissible harmonic Ritz value set for GMRES with stagnation. In this section we will show that any admissible harmonic Ritz value set is possible for given GMRES residual norms.

By Propositions 2.1 and 2.2, given GMRES residual norms implies entries of \( Q \) are uniquely determined up to complex signs. Given an admissible harmonic Ritz value set \( \Theta \), by constructing a desirable nonsingular upper triangular matrix \( R \) (see the approach below), we can obtain a pair \( \{ H, e_1 \} \), for which GMRES produces harmonic Ritz value set \( \Theta \) and the prescribed residual norms.

Now we describe how to construct \( R \). At step \( k \), let \( \{ \tilde{r}_{jk} \}_{j=1}^{k} \) denote the entries of the last column of \( R^{-1} - 1 \).

(i) If \( Q_k \) is nonsingular, we consider the parameterized inverse eigenvalue problem for prescribed harmonic Ritz values: Given \( k \) nonzero complex number (harmonic Ritz values) \( \theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_k^{(k)} \), and two matrices \( Q_k, R_{k-1}^{-1} \); find \( \{ \tilde{r}_{jk} \}_{j=1}^{k} \) such that

\[
\begin{bmatrix} 1 \\ \theta_1^{(k)} \\ \theta_2^{(k)} \\ \vdots \\ \theta_k^{(k)} \end{bmatrix}
\]

is the spectrum of the matrix

\[
Q_k^* R_k^{-1} = Q_k^* \begin{bmatrix} R_{k-1}^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \sum_{j=1}^{k} \tilde{r}_{jk} Q_k^* e_j e_k^*.
\]

Note that the \( k \) matrices \( Q_k^* e_j e_k^* \) \( (1 \leq j \leq k) \) are linearly independent and

\[
\text{tr}(Q_k^* e_1 e_1^*) = q_1, k \neq 0.
\]

Helton et. al [7] proved that almost all such parameterized inverse eigenvalue problems are solvable.

(ii) If \( Q_k \) is singular, which means GMRES stagnates at step \( k \), by Proposition 2.4, we can set \( \tilde{r}_{jk} = 0 \) for \( j = 1 : k-1 \) and \( \tilde{r}_{kk} = 1 \).

Once all \( \{ \tilde{r}_{jk} \}_{j=1}^{k} \) for \( k = 1 : n \) are found, we obtain \( R^{-1} \), then \( H \) follows by \( H = QR \). GMRES applied to \( \{ H, e_1 \} \) produces the prescribed harmonic Ritz values.
(in all steps) and the prescribed residual norms. That is to say, any admissible harmonic Ritz value set is possible for given GMRES residual norms.

**Remark 3.1.** Given $Q$ and $R_{k-1}$, we provide an obvious approach for construction of $R_k$. It is sufficient to consider the case $Q_k$ is nonsingular. We obtain \( \{r_{jk}\}_{j=1}^k \), the entries of the last column of $R_k$, by solving the following linear system

\[
\det(R_k - \theta_i^{(k)} Q_k^*) = 0, \quad i = 1 : k.
\]

**REFERENCES**

[1] M. Arioli, V. Pták, and Z. Strakoš, Krylov sequences of maximal length and convergence of GMRES, BIT, 38 (1998), pp. 636–643.

[2] W. E. Arnoldi, The principle of minimized iteration in the solution of the matrix eigenvalue problem, Quart. Appl. Math., 9 (1951), pp. 17–29.

[3] Jurjen Duintjer Tebbens and Gérard Meurant, Any Ritz value behavior is possible for Arnoldi and for GMRES, SIAM J. Matrix Anal. Appl., 33 (2012), pp. 958–978.

[4] Roland W. Freund, Quasi-kernel polynomials and their use in non-Hermitian matrix iterations, J. Comput. Appl. Math., 43 (1992), pp. 135–158.

[5] Jurjen Duintjer Tebbens and Gérard Meurant, Any Ritz value behavior is possible for Arnoldi and for GMRES, SIAM J. Matrix Anal. Appl., 33 (2012), pp. 958–978.

[6] Anne Greenbaum, Vlastimil Pták, and Zdeněk Strakoš, Any nonincreasing convergence curve is possible for GMRES, SIAM J. Matrix Anal. Appl., 17 (1996), pp. 465–469.

[7] Anne Greenbaum, Vlastimil Pták, and Zdeněk Strakoš, Matrices that generate the same Krylov residual spaces, in Recent advances in iterative methods, vol. 60 of IMA Vol. Math. Appl., Springer, New York, 1994, pp. 95–118.

[8] William Helton, Joachim Rosenthal, and Xiaochang Wang, Matrix extensions and eigenvalue completions, the generic case, Trans. Amer. Math. Soc., 349 (1997), pp. 3401–3408.

[9] Gérard Meurant, GMRES and the Arioli, Pták, and Strakoš parametrization, BIT, 52 (2012), pp. 687–702.

[10] Youcef Saad and Martin H. Schultz, GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 856–869.