On Harmonic Ritz vectors and the stagnation of GMRES

Mashetti Ravibabu

Indian Institute of Science, Bengaluru, India

Abstract

This paper derives a necessary and sufficient condition for the coincidence of Harmonic residual vectors and the residual vector in GMRES. The properties of the harmonic Ritz values at the stagnation of GMRES were described in the Proposition-4.2 of [1]. Necessary and sufficient conditions basing on Harmonic Ritz vectors for the stagnation have derived in this paper.

Keywords: GMRES, Harmonic Ritz vectors, Stagnation

1. Introduction

The GMRES method is widely used for approximating the solution of sparse nonsymmetric linear system of equations; see [4]. GMRES arbitrarily chooses an initial residual vector \( r_0 \), and then at each iteration updates a residual vector using the Krylov subspace that based on \( r_0 \) and the coefficient matrix \( A \). Thus a residual vector can be written as the polynomial in \( A \), so-called the residual polynomial acting on \( r_0 \).

The zeroes of the residual polynomial are the Harmonic Ritz values [2]. Harmonic Ritz values are approximations to eigenvalues of \( A \) from the Krylov subspace in GMRES. The corresponding residual vectors, so-called Harmonic Residual vectors are orthogonal to the \( A \) image of the Krylov subspace in GMRES.

If a residual vector of the linear system remains the same for a few consecutive iterations of GMRES then it is called the stagnation. The relations between Harmonic Ritz values in any two successive iterations during the stagnation have derived in this paper.
stagnation are given in the Proposition-4.2 of [1]. This paper shows that the coincidence of GMRES residual vector and harmonic residual vectors is theoretically possible. Then, it derives a necessary and sufficient condition for the stagnation of GMRES based on the Harmonic Ritz vectors. It also discusses the preserve of harmonic Ritz vectors during the stagnation phase of GMRES.

The paper is organized as follows: Section 2 introduces the GMRES method. In Section 3 a least squares problem is devised that connects solutions of least squares problems in any two successive iterations of GMRES. Using the results of Section-3, Section 4 derives a necessary and sufficient condition for the coincidence of the residual and Harmonic residual vectors. Then Section 5 derives a necessary and sufficient condition for the stagnation of GMRES. Section 6 concludes the paper.

2. GMRES

Consider the following system of linear equations:

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

Let $$x_0 \in \mathbb{C}^n$$ be an arbitrarily chosen initial approximation to the solution of the above problem. Without loss of generality, we assumed throughout the paper that $$x_0 = 0$$ so that the initial residual vector is $$r_0 = b$$. Then, at the $$i^{th}$$ iteration of GMRES an approximate solution belongs to the Krylov subspace:

$$\mathcal{K}_i(A, b) = \text{span}\{b, Ab, \ldots, A^{i-1}b\}$$

and is of minimal residual norm:

$$\|r_i\| = \min_{x \in \mathcal{K}_i(A, b)} \|b - Ax\|. \quad (2.1)$$

GMRES solves this minimization problem using the following Arnoldi recurrence relation:

$$AV_i = V_i H_i + h_{i+1,i}v_{i+1}e_i^*, \quad \text{where} \quad v_1 = \frac{b}{\|b\|}, \quad (2.2)$$

where the matrix $$V_i = [v_1 \ v_2 \ \cdots \ v_i]$$, and $$H_i$$ is an unreduced upper Hessenberg matrix of order $$i$$. The vectors $$\{v_1, v_2, \cdots, v_j\}$$ form an orthonormal
basis for \( K_j(A, b) \), for \( j = 1, 2, \ldots, i \). A vector \( v_{i+1} \) is of unit norm, and is orthogonal to \( v_j \) for \( j \leq i \).

GMRES uses the equation (2.2) to recast the least squares problem in (2.1) into the following:

\[
z_i = \arg\min_{x \in \mathbb{C}^i} \| b - AV_i x \| = \arg\min_{x \in \mathbb{C}^i} \| \beta V_{i+1} e_1 - V_{i+1} \hat{H} i x \|, \tag{2.3}
\]

where \( \beta = \| b \| \), and \( \hat{H} i \) is an upper Hessenberg matrix obtained by appending the row \( [0 \ 0 \ \cdots \ h_{i+1,i}] \) at the bottom of the matrix \( H_i \). As columns of the matrix \( V_{i+1} \) are orthonormal, the above least squares problem is equivalent to the following problem:

\[
z_i = \arg\min_{x \in \mathbb{C}^i} \| \beta e_1 - \hat{H} i x \|.
\]

GMRES solves this problem for the vector \( z_i \) by using the QR decomposition of the matrix \( \hat{H} i \). From the equation (2.3) note that a vector \( z_i \) satisfies the following normal system of equations:

\[
V_i^* A^* AV_i z_i = V_i^* A^* b = \beta V_i^* A^* V_i e_1. \tag{2.4}
\]

Since the columns of \( V_i \) are orthonormal, and \( v_{i+1} \) is orthogonal to the columns of \( V_i \), by using the equation (2.2), the above equation can be rewritten as follows in the terms of \( H_i \):

\[
(H_i^* H_i + |h_{i+1,i}|^2 e_i e_i^*) z_i = \beta H_i^* e_1. \tag{2.5}
\]

From the equation (2.1) note that the norm of a residual vector associated with \( V_i z_i \) is smaller over the Krylov subspace of dimension \( i \).

3. The new Least Squares problem

In this section, we devise a least squares problem that connects approximate solutions at two successive iterations of GMRES. Throughout this section, iteration number is fixed at \( m \), and \( y \) denotes the solution of a least squares problem in the equation (2.3), for \( i = m \).

Consider the following least squares problem:

\[
z = \arg\min_{x \in \mathbb{C}^m} \| b - AV_m (I - e_m e_m^*) x \|.
\]
Note that a solution vector \( z \) of this least squares problem satisfies the following system of normal equations:

\[
(I - e_me_m^*)(V_mA^*(b - AV_m(I - e_me_m^*)z)) = 0. \tag{3.1}
\]

As linear span of a vector \( e_m \) is the null space of a projection operator \( (I - e_me_m^*) \), it gives the following:

\[
V_m^*A^*(b - AV_m(I - e_me_m^*)z) = Ke_m,
\]

where \( K \) is a scalar that can be obtained by applying an inner product with a vector \( e_m \) on both the sides of the above equation. The next theorem makes a connection between solutions of a new least squares problem and the usual least squares problem of GMRES for the vector space spanned by columns of \( V_{m-1} := [v_1 v_2 \cdots v_{m-1}] \).

**Theorem 1.** Let a vector \( z \) be the same as in the equation \( \text{(3.1)} \), and \( z_{m-1} \) be a vector of length \( m - 1 \) such that \( V_m(I - e_me_m^*)z = V_{m-1}z_{m-1} \). Then

\[
z_{m-1} = \arg \min_{x \in \mathbb{C}^{m-1}} \| b - AV_{m-1}x \|^2 \tag{3.2}
\]

**Proof.** From the equation \( \text{(3.1)} \) we have

\[
(I - e_me_m^*)V_m^*A^*AV_m(I - e_me_m^*)z = (I - e_me_m^*)V_m^*A^*b.
\]

On substituting \( V_m(I - e_me_m^*)z = V_{m-1}z_{m-1} \) the previous equation gives

\[
(I - e_me_m^*)V_m^*A^*AV_{m-1}z_{m-1} = (I - e_me_m^*)V_m^*A^*b. \tag{3.3}
\]

As linear span of a vector \( e_m \) is the null space of a projection operator \( (I - e_me_m^*) \), this equation gives the following for some scalar \( K \):

\[
V_m^*A^*(b - AV_{m-1}z_{m-1}) = Ke_m. \tag{3.4}
\]

Thus the vector \( V_m^*A^*(b - AV_{m-1}z_{m-1}) \) is parallel to the vector \( e_m \). Since \( e_i^*e_m = 0 \) for \( i = 1, 2, \ldots, m - 1 \), the above equation gives

\[
V_{m-1}^*A^*A(b - AV_{m-1}z_{m-1}) = 0.
\]

Therefore, the vector \( z_{m-1} \) is a solution of the least squares problem in \( \text{(3.2)} \). Hence, the theorem proved.
Observe from the equation (3.4) that \( K = v^*_m A^* r_{m-1} = < Av_m, r_{m-1} > \), where \( r_{m-1} = b - AV_{m-1} z_{m-1} \). The next theorem relates an approximate solution at the \( m^{th} \) iteration of GMRES to residual norms in the \((m - 1)^{th}\) and \( m^{th} \) iterations.

**Theorem 2.** Let \( r_{m-1} \) and \( r_m \) be residual vectors at \((m - 1)^{th}\) and \( m^{th}\) iterations of GMRES, respectively. Assume that column vectors of the matrix \( AV_m \) are linearly independent. If a vector \( y \) is the solution of the least squares problem at \( m^{th} \) iteration of GMRES then

\[
\| r_{m-1} \|^2 - \| r_m \|^2 = Ke^*_m y.
\]

**Proof.** From the hypothesis of the theorem we have \( V_m^* A^* AV_m y = V_m^* A^* b \). Observe that by using this, the equation (3.4) gives

\[
V_m^* A^* AV_m (y - (z_{m-1} 0)) = Ke_m.
\]

As column vectors of the matrix \( AV_m \) are linearly independent the above equation gives the following:

\[
y - (z_{m-1} 0) = K (V_m^* A^* AV_m)^{-1} e_m. \tag{3.5}
\]

This implies

\[
AV_m (y - (z_{m-1} 0)) = K AV_m (V_m^* A^* AV_m)^{-1} e_m,
\]

and

\[
r_{m-1} - r_m = K AV_m (V_m^* A^* AV_m)^{-1} e_m. \tag{3.6}
\]

In the above equation we used the relations \( r_m = b - AV_m y \), and the following:

\[
r_{m-1} = b - AV_{m-1} z_{m-1} = b - AV_m (z_{m-1} 0).
\]

Now, apply an inner product with \( r_0 = b \) on both the sides of the equation (3.6). It gives

\[
r_{m-1}^* r_0 - r_m^* r_0 = K e_m^* (V_m^* A^* AV_m)^{-1} V_m^* A^* b. \tag{3.7}
\]
By using $V_m^*A^*AV_my = V_m^*A^*b$, observe that the right-hand side expression in the above equation is $Ke_m^*y$. The proof will be complete if

$$r_{m-1}^*r_0 - r_m^*r_0 = \|r_{m-1}\|^2 - \|r_m\|^2.$$  

From the Theorem we know that $r_{m-1} = b - AV_{m-1}z_{m-1}$ is orthogonal to $AV_{m-1}z_{m-1} = r_{m-1} - b = r_{m-1} - r_0$. Similarly, the residual vector $r_m$ is orthogonal to $r_m - r_0$. Thus, $r_i^*r_0 = \|r_i\|^2$ for $i = m - 1, m$. Therefore, the above equation holds true, and the proof is over.

4. Equality of Residual and Harmonic Residual vectors

In this section, we define Harmonic Residual vectors and will discuss the coincidence of these vectors with a residual vector in GMRES. As in the previous section, we fix iteration number in GMRES as $m$ and will use the notation of the Section-2.

Definition 1. The $m$ eigenvalues $\{\sigma_j\}_{j=1}^m$ of the generalized eigenvalue problem

$$V_m^*A^*AV_mu = \sigma V_m^*A^*V_mu$$

are called the Harmonic Ritz values at iteration $m$ of GMRES. The vectors $\{u_j\}_{j=1}^m$ are called the Harmonic Ritz vectors. The pair $(\sigma, u)$ is called the Harmonic Ritz pair.

Definition 2. Let $(\sigma, u)$ be a Harmonic Ritz pair at iteration $m$ of GMRES. The vector $AV_mu - \sigma V_mu$ is called the Harmonic residual vector at iteration $m$ of GMRES.

The following theorem derives a necessary condition for the equality of a Harmonic residual vector $AV_mu - \sigma V_mu$ and $b - AV_my$, the residual vector at $m$th iteration of GMRES.

Theorem 3. Let a Harmonic residual vector $AV_mu - \sigma V_mu$ be the same as the residual vector $b - AV_my$ at $m$th iteration of GMRES. Then $e_m^*y = -e_m^*u$.

Proof. Consider $AV_mu - \sigma V_mu = b - AV_my$. By using $b = \beta V_m e_1$ and the equation (2.2) for $i = m$, this implies

$$V_mH_mu + h_{m+1,m}m_{m+1}^*e_m^*u - \sigma V_mu = \beta V_m e_1 - V_m H_my - h_{m+1,m}m_{m+1}^*y.$$  

Recall that columns of the matrix \( V_m \) form an orthonormal basis for the Krylov subspace \( \mathcal{K}_m(A, b) \). As \( v_{m+1} \) is orthogonal to column vectors of \( V_m \), the above equation implies the following:

\[
H_m u - \sigma u = \beta e_1 - H_m y \quad \text{and} \quad e_m^* u = -e_m^* y.
\]

Hence, the theorem proved.

In what follows, we prove that \( e_m^* y = -e_m^* u \) is a sufficient condition for the equality of the vectors in the Theorem 3.

**Theorem 4.** Let \( AV_m u - \sigma V_m u \) be a Harmonic residual vector, and \( b - AV_m y \) be the residual vector at \( m^{th} \) iteration of GMRES. Assume that there is no stagnation at \( m^{th} \) iteration, and \( e_m^* y = -e_m^* u \). Then \( AV_m u - \sigma V_m u = b - AV_m y \).

**Proof.** As \((\sigma, u)\) is a Harmonic Ritz pair, by using the Definition 1 and the equation (2.2) for \( i = m \), it satisfy the following equation:

\[
H_m^* H_m u + |h_{m+1, m}|^2 e_m e_m^* u = \sigma H_m^* u.
\]  

(4.1)

Similarly, as \( b - AV_m y \) is the residual vector at \( m^{th} \) iteration, by using the equation (2.5) for \( i = m \), the vector \( y \) satisfies the following equation:

\[
(H_m^* H_m + |h_{m+1, m}|^2 e_m e_m^*) y = \beta H_m^* e_1.
\]

(4.2)

By using \( e_m^* y = -e_m^* u \), the above two equations imply the following relation:

\[
H_m^* (H_m u - \sigma u + H_m y - \beta e_1) = 0.
\]

As there is no stagnation at \( m^{th} \) iteration, by using the Lemma 11 and the Theorem 4 from the Section 4, observe that \( H_m^* \) is a non-singular matrix. Thus, the above equation implies \( H_m u - \sigma u = \beta e_1 - H_m y \). On multiplying both the sides with a matrix \( V_m \) gives \( V_m H_m u - \sigma V_m u = \beta V_m e_1 - V_m H_m y \). Now, by using the equation (2.5) for \( i = m \), this equation can be rewritten as follows:

\[
AV_m u - h_{m+1, m} v_{m+1} e_m^* u - \sigma V_m u = \beta V_m e_1 - AV_m y + h_{m+1, m} v_{m+1} e_m^* y.
\]

As \( \beta V_m e_1 = b \) and \( e_m^* y = -e_m^* u \), this gives \( AV_m u - \sigma V_m u = b - AV_m y \), the required equation. Hence, the proof is over.
Observe that the Theorems 3 and 4 can be generalized to the following:

**Theorem 5.** Let $AV_mu - \sigma V_mu$ be a Harmonic residual vector, and $b - AV_my$ be the residual vector at $m^{th}$ iteration of GMRES. Assume that there is no stagnation at $m^{th}$ iteration. Then for some non-zero scalar $K$, $AV_mu - \sigma V_mu = K(b - AV_my)$, if and only if $e^*_m u = -K(e^*_m y)$.

The proof of theorem 5 is trivial from the proofs of the Theorems 3 and 4. The following example illustrates the Theorem 5.

**Example 1.** Consider the system of equations $Ax = b$, where

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix},$$

and $b = [1 0 0]' = e_1$. Similarly, we use $e_2$ and $e_3$ to represent the vectors $[0 1 0]'$ and $[0 0 1]'$ respectively. Let the zero vector be an approximate solution so that $e_1$ is the initial residual vector $r_0$ in GMRES.

Starting with $e_1$, for the matrix $A$ the Arnoldi algorithm gives the following after 2 iterations:

$$AV_2 = V_2 H_2 + e_3 [0 \ 1]$$

where $V_2 = [e_1, e_2]$, and

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}.$$

The residual vector at the 2nd iteration of GMRES is

$$r_2 = b - AV_2 [1/3 \ 1/3]' = [1/3 \ -1/3 \ -1/3]' .$$

This example do not have the stagnation of GMRES. The harmonic Ritz values at 2nd iteration of GMRES are $\pm \sqrt{3}$, and $V_2 [\sqrt{3}/2 \ 1/2]' = [\sqrt{3}/2 \ 1/2 \ 0]'$ is the harmonic Ritz vector corresponding to $\sqrt{3}$. Thus, the corresponding harmonic residual vector is

$$A \begin{bmatrix} \sqrt{3}+1 \\ 1/2 \\ 0 \end{bmatrix} - \sqrt{3} \begin{bmatrix} \sqrt{3}+1 \\ 1/2 \\ 0 \end{bmatrix} = \begin{bmatrix} -1/2 \\ 1/2 \\ 1/2 \end{bmatrix} .$$

Observe that for this example the above vector is equal to $\frac{\sqrt{3}}{2} \times r_2$, and $e_2^* u = 1/2$, $e_2^* y = 1/3$. Therefore, the vectors $u$ and $y$ satisfy the necessary and sufficient condition in the Theorem 5.
Theorem 4 has given a sufficient condition in the absence of the stagnation for the coincidence of a Harmonic residual vector and the residual vector of GMRES at the $m^{th}$ iteration. The following theorem discusses this coincidence of vectors in the presence of the stagnation. We delay its proof to the next section for the convenience.

**Theorem 6.** Let $AV_m u - \sigma V_m u$ be a Harmonic residual vector, and $b - AV_m y$ be the residual vector at $m^{th}$ iteration of GMRES. Assume that there is a stagnation at $m^{th}$ iteration. Then $AV_m u - \sigma V_m u = b - AV_m y + \xi V_m s_2$, where $s_2$ is a vector such that $V_m^* A^* V_m s_2 = 0$, and $\xi$ is some scalar.

5. **The stagnation of GMRES**

This section derives a necessary and sufficient condition on harmonic Ritz vectors for the stagnation of GMRES. For this, it first derives a necessary and sufficient condition on $H_m$, when residuals at $(m - 1)^{th}$ and $m^{th}$ iterations of GMRES are stagnated, that means $\|r_{m-1}\| = \|r_m\|$. From the Theorem 2, observe that this happens if and only if $K = 0$ or $e_m^* y = 0$. The next theorem shows that if either $K$ or $e_m^* y$ is zero, then the other one also equal to the zero.

**Lemma 1.** Let a scalar $K$ and a vector $y$ be the same as in the Theorem 2. Then, $K = 0$ if and only if $e_m^* y = 0$.

**Proof.** First we prove $e_m^* y = 0$, if $K = 0$. By using the equation (3.5), note that $K = 0$ implies

$$y = \begin{pmatrix} z_{m-1} \\ 0 \end{pmatrix}.$$  

Recall that $z_{m-1}$ is a vector of length $(m - 1)$. Therefore, $e_m^* y = 0$. Next, we prove the converse, that means, $K = 0$ if $e_m^* y = 0$. By using the equation (3.5), observe that $e_m^* y = 0$ implies

$$Ke_m^* (V_m^* A^* V_m)^{-1} e_m = 0.$$  

As column vectors of the matrix $AV_m$ are linearly independent, the matrix $(V_m^* A^* V_m)^{-1}$ is a positive definite matrix. Therefore, this implies $K = 0$. Hence, the proof is over.

By using the Lemma 1, the following theorem proves that the stagnation at $m^{th}$ iteration of GMRES occurs if and only if $H_m$ is a singular matrix.
Theorem 7. Let the vectors $r_{m-1}, r_m$ and $y$ be the same as in the Theorem 2, and $H_m$ is an upper Hessenberg matrix at $m^{th}$ iteration of GMRES. Assume that $r_{m-1} \neq 0$. Then $e^*_my = 0$ if and only if $H_m$ is a singular matrix.

Proof. Let $e^*_my = 0$. By using the equation (2.5) for $i = m$, this gives the following equation:

$$H^*_mH_my = \beta H^*_me_1.$$

(5.1)

If $H_m$ is non-singular, this equation implies $H_my = \beta e_1$, and $y = \beta H^{-1}_me_1$. This together with the equation (2.2) gives

$$r_m = b - AV_my = b - V_mH_my - h_{m+1,m}e_{m+1}^*y = b - \beta V_me_1 - h_{m+1,m}e_{m+1}^*y. $$

By using the fact that $b = \beta V_me_1$, and $e^*_my = 0$, this gives $r_m = 0$. Further, the Theorem 2 implies $r_{m-1} = 0$, a contradiction to the hypothesis of the theorem that $r_{m-1} \neq 0$. Therefore, $H_m$ is a singular matrix.

Now, we prove the converse. Let $H_m$ be a singular matrix. Then there exists a non-zero vector $s$ such that $H_ms = 0$. As $H_m$ is an unreduced upper Hessenberg matrix this implies

$$e^*_ms \neq 0.$$

Otherwise, $H_ms = 0$ implies $s = 0$. Now, take an inner product with $s$ on both the sides of the equation (2.2) for $i = m$. This gives

$$s^*H^*_mH_my + |h_{m+1,m}|^2s^*e_me^*_my = \beta s^*H^*_me_1.$$

By using $H_ms = 0$ and $e^*_ms \neq 0$, this equation implies $e^*_my = 0$. Therefore, the theorem proved.

\[ \Box \]

The following theorem derives a necessary and sufficient condition on harmonic Ritz vectors for the stagnation at $m^{th}$ iteration of GMRES. For this, it uses the Lemma 1 and the Theorem 7.

Theorem 8. Let $(\sigma, u)$ be a harmonic Ritz pair at $m^{th}$ iteration of GMRES. Assume that $b - AV_my$ is the residual vector at the same iteration. If $e^*_my = 0$ then $e^*_mu = 0$.

Proof. Let $e^*_my = 0$. The proof for $e^*_mu = 0$ is required. As $e^*_my = 0$ from the Lemma 1 and the Theorem 7 note that $H_m$ is a singular matrix. Assume that $H_m$ is of the following form:

$$H_m := \begin{bmatrix} H_{m-1} & h \\ \gamma e^*_{m-1} & \alpha \gamma \end{bmatrix},$$

(5.2)
where $H_{m-1}$ is a principal submatrix of order $m - 1$ from the top left corner of $H_m$. The singularity of a matrix $H_m$ implies the existence of a vector $s_1$ such that

$$h = H_{m-1}s_1.$$ 

As $(\sigma, \mu)$ is a harmonic Ritz pair, it satisfies the equation (4.1). By using the form of a matrix $H_m$ in the above equation, (4.1) can be written as follows:

$$
\begin{bmatrix}
H_{m-1}^*H_{m-1} + |\gamma|^2e_{m-1}e_{m-1}^* & H_{m-1}^*h + \alpha|\gamma|^2e_{m-1} \\
h^*H_{m-1} + \bar{\alpha}|\gamma|^2e_{m-1} & h^*h + |\alpha\gamma|^2
\end{bmatrix}u = \\
\sigma
\begin{bmatrix}
H_{m-1}^* \\
h^*
\end{bmatrix}
\begin{bmatrix}
\bar{\gamma}e_{m-1} \\
\bar{\alpha}\gamma
\end{bmatrix}u - |h_{m+1,m}|^2e_me_mu. 
$$

(5.3)

Assume that $u_{1:m-1}$ represents a vector whose entries are the same as first $m - 1$ elements of a vector $u$, and $u_m$ denotes a last entry of the vector $u$. Following this notation, the comparison of both the sides of the above equation gives the following relations:

$$H_{m-1}^*H_{m-1}u_{1:m-1} - \sigma H_{m-1}^*u_{1:m-1} + |\gamma|^2e_{m-1}(e_{m-1}^*u_{1:m-1}) = u_m(\sigma\bar{\gamma}e_{m-1} - H_{m-1}^*h - \alpha|\gamma|^2e_{m-1}), \quad (5.4)$$

and

$$h^*H_{m-1}u_{1:m-1} + \bar{\alpha}|\gamma|^2e_{m-1}u_{1:m-1} + (h^*h + |\alpha\gamma|^2)u_m = \\
\sigma h^*u_{1:m-1} + \sigma\bar{\alpha}\gamma u_m - |h_{m+1,m}|^2u_m.$$ 

On substituting $h = H_{m-1}s_1$, this implies

$$s_1^*(H_{m-1}^*H_{m-1} - \sigma H_{m-1}^*)u_{1:m-1} + \bar{\alpha}|\gamma|^2e_{m-1}u_{1:m-1} + (h^*h + |\alpha\gamma|^2 - \sigma\bar{\alpha}\gamma + |h_{m+1,m}|^2)u_m = 0.$$ 

As $H_m$ is an unreduced upper Hessenberg singular matrix, from the equations (5.2) and $h = H_{m-1}s_1$, note that $\alpha$ and $\gamma$ are non-zero, and $\bar{\alpha} = s_1^*e_{m-1}$. Further, apply an inner product on both the sides of the equation (5.4) with a vector $s_1$. Then, substituting it in the above equation gives

$$u_m(\sigma\bar{\gamma}s_1^*e_{m-1} - h^*h - |\alpha\gamma|^2 + h^*h + |\alpha\gamma|^2 - \sigma\bar{\alpha}\gamma + |h_{m+1,m}|^2) = 0. \quad (5.5)$$

The above equation has used the relation $h = H_{m-1}s_1$ to obtain the second term inside the parentheses. Using $\bar{\alpha} = s_1^*e_{m-1}$ and $h_{m+1,m} \neq 0$ observe that the term inside the parentheses of the equation (5.3) is non-zero. Therefore, $u_m := e_m^*u = 0$. Hence, the theorem proved. \hfill \Box
Observe that in the Theorem-8 $\sigma \neq 0$ is not necessary as the equation (5.5) holds true for $\sigma = 0$ as well. Next, the following theorem proves the converse of the Theorem-8.

**Theorem 9.** Let vectors $u$ and $y$ be the same as in the Theorem-8. If $e^*_mu = 0$ then $e^*_my = 0$.

**Proof.** As $(\sigma, u)$ is a harmonic Ritz pair, it satisfies the equation (4.1). Further, using $e^*_mu = 0$ it gives $H^*_mH_mu = \sigma H^*_mu$. This implies either $H_mu - \sigma u$ is a zero vector or $H_m$ is a singular matrix. Assume that $H_mu - \sigma u$ is a zero vector. Then, as $H_m$ is an unreduced upper Hessenberg matrix and $e^*_mu = 0$, by using the Lemma-2.1 in [3], the equation $H_mu = \sigma u$ implies $u$ is a harmonic Ritz vector. Therefore, $H_m$ is a singular matrix. Now, by using the Theorem-7 this gives $e^*_my = 0$. Hence, the proof is over.

The Theorems-1, 8, and 9 have shown that the stagnation occurs at $m$th iteration of GMRES if and only if $e^*_mu = 0$ and $e^*_my = 0$. That means, when the stagnation occurs, the necessary and sufficient condition in the Theorems-3 and 4 for the coincidence of a harmonic residual vector and the residual vector in GMRES is trivial. The following is the proof for the Theorem-6 of the previous section.

**Proof of Theorem-6.** As $(\sigma, u)$ is a harmonic Ritz pair, and $b - AV_my$ is a residual at $m$th iteration, the vectors $u$ and $y$ satisfy the equations (4.1) and (4.2) respectively. Since there is a stagnation at $m$th iteration of GMRES, the Theorems-1, 8, and 9 imply $e^*_mu = 0$ and $e^*_my = 0$. Thus, $H^*_mH_mu = \sigma H^*_mu$, and $H^*_mH_my = \beta H^*_me_1$. These two equations together imply $H^*(H_mu - \sigma H^*_mu + H_my - \beta H^*_me_1) = 0$. This implies

$$H_mu - \sigma u = \beta e_1 - H_my + \xi s_2.$$  

Here, $\xi$ is a scalar, and $s_2$ is a vector such that $H^*_ms_2 = 0$. Note that a vector $s_2$ exists due to the Theorem-7 and the stagnation of GMRES. On multiplying both the sides of the above equation with a matrix $V_m$ gives $V_mH_mu - \sigma V_mu = \beta V_me_1 - V_my + \xi V_ms_2$. Now, by using $e^*_mu = 0, e^*_my = 0$, and the equation (2.5) for $i = m$, this equation can be written as follows:

$$AV_mu - \sigma V_mu = \beta V_me_1 - AV_my + \xi V_ms_2$$

As $\beta V_me_1 = b$, this gives $AV_mu - \sigma V_mu = b - AV_my + \xi V_ms_2$, the required equation. Hence, the proof is over. \qed
In the following, we prove the theorems those relate harmonic Ritz vectors at any two successive iterations of GMRES in the presence of the stagnation.

**Lemma 2.** Assume that the stagnation has occurred at the $m^{th}$ iteration of GMRES. Let $u$ be a harmonic Ritz vector corresponding to the non-zero harmonic Ritz value $\sigma$, at $m^{th}$ iteration. Then $(\sigma, u_{1:m-1})$ is a harmonic Ritz pair at $(m-1)^{th}$ iteration of GMRES.

**Proof.** Due to the stagnation at $m^{th}$ iteration of GMRES the Lemma-1 and the Theorem-8 give $e^*_m u = 0$. Substituting this in the equation (5.4) gives the desired result, that means $(\sigma, u_{1:m-1})$ is a harmonic Ritz pair at $(m-1)^{th}$ iteration.

Next, in the following, we prove the converse of the Lemma-2.

**Lemma 3.** Let $u$ be a harmonic Ritz vector corresponding to the non-zero harmonic Ritz value $\sigma$, at $m^{th}$ iteration. If $(\sigma, u_{1:m-1})$ is a harmonic Ritz pair at $(m-1)^{th}$ iteration of GMRES then there is a stagnation at $m^{th}$ iteration of GMRES.

**Proof.** From the hypothesis of the lemma and the equation (5.4) we have $e^*_m u = 0$. By using the Theorem-9 this gives $e^*_m y = 0$. Now, use the Theorem-2 to conclude $r_{m-1} = r_m$, where $r_i$ is a residual at the $i^{th}$ iteration. Therefore, there is a stagnation at $m^{th}$ iteration. Hence, the proof is over.

6. **Conclusions**

This paper shows that coincidence of the GMRES residual vector and Harmonic residual vector is theoretically possible, and derives the necessary and sufficient condition for this coincidence. Then, for the stagnation in GMRES, it derives necessary and sufficient conditions those based on elements of a harmonic Ritz vector. Further, it shows that in case of the stagnation, the harmonic Ritz vectors corresponding to non-zero harmonic Ritz values are preserved. The procedure followed in this paper for proving these results will be helpful for the study of the near stagnation of GMRES in terms of elements of harmonic Ritz vectors.

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