



A New Implementation of GMRES Using Generalized Purcell Method

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Abstract

In this paper, a new method based on the generalized Purcell method is proposed to solve the usual least-squares problem arising in the GMRES method. The theoretical aspects and computational results of the method are provided. For the popular iterative method GMRES, the decomposition matrices of the Hessenberg matrix is obtained by using a simple recursive relation instead of Givens rotations. The other advantages of the proposed method are low computational cost and no need for orthogonal decomposition of the Hessenberg matrix or pivoting. The comparisons for ill-conditioned sparse standard matrices are made. They show a good agreement with available literature.

Keywords: Generalized Purcell method; Krylov subspace methods; weighted minimal residual method; generalized Purcell minimal residual method; Ill-conditioned problems

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1. Introduction

The generalized minimal residual (GMRES) method is a popular iterative method for solving a linear system of n equations for the n variables, which can be written in the form

$$A\mathbf{x} = \mathbf{b}. \quad (1)$$

This method is based on Arnoldi's process (Arnoldi, 1951), which is a version of the Gram-Schmidt method tailored to Krylov subspaces $K_k(A, \mathbf{r}_0)$, i.e.,

$$K_k(A, \mathbf{r}_0) = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{k-1}\mathbf{r}_0\}. \quad (2)$$

The construction of the subspace $K_k(A, \mathbf{r}_0)$ starts with an initial guess $\mathbf{r}_0 = \mathbf{b}$ and generates an approximate solution \mathbf{x}_k such that

$$\mathbf{x}_k = \text{argmin}_{\mathbf{x} \in K_k(A, \mathbf{r}_0)} \|\mathbf{Ax} - \mathbf{b}\|_2. \quad (3)$$

Starting with the normalized right-hand side $\mathbf{v}_1 = \frac{\mathbf{r}_0}{\|\mathbf{r}_0\|_2}$ as a basis for $K_1(A, \mathbf{r}_0)$, Arnoldi's process recursively builds an orthonormal basis for $K_{k+1}(A, \mathbf{r}_0)$ by orthogonalizing the vector $A\mathbf{v}_k$ from $K_{k+1}(A, \mathbf{r}_0)$ to the previous space $K_k(A, \mathbf{r}_0)$, i.e.,

$$\mathbf{v}_{k+1} = A\mathbf{v}_k - (h_{1k}\mathbf{v}_1 + \dots + h_{kk}\mathbf{v}_k),$$

where $h_{ik} = \mathbf{v}_i^* A\mathbf{v}_k$. The new basis vector is defined as $\mathbf{v}_{k+1} = \frac{A\mathbf{v}_k - \sum_{i=1}^k h_{ik}\mathbf{v}_i}{\|A\mathbf{v}_k - \sum_{i=1}^k h_{ik}\mathbf{v}_i\|_2}$. If we collect the orthonormal basis vectors for $K_k(A, \mathbf{r}_0)$ in a matrix form, say $V_k = [\mathbf{v}_1, \dots, \mathbf{v}_k]$, then the decomposition associated with Arnoldi's process is $AV_k = V_{k+1}H_k$, where $H_k = [h_{ij}]$ is a $(k+1)$ -by- k upper Hessenberg matrix. Here, it should be noted that $h_{k+1,k} = \|\mathbf{v}_{k+1}\|_2$.

Every solution $\mathbf{x} \in K_k(A, \mathbf{r}_0)$ in the context of the linear least squares problem (3) starting with $\mathbf{r}_0 = \mathbf{b}$ implies that for some \mathbf{y} we have $\mathbf{x} = V_k\mathbf{y}$ and

$$\begin{aligned} \min_{\mathbf{x} \in K_k(A, \mathbf{b})} \|\mathbf{Ax} - \mathbf{b}\|_2 &= \min_{\mathbf{y}} \|AV_k\mathbf{y} - \beta V_{k+1}\mathbf{e}_1\|_2 \\ &= \min_{\mathbf{y}} \|V_{k+1}H_k\mathbf{y} - \beta V_{k+1}\mathbf{e}_1\|_2 \\ &= \min_{\mathbf{y}} \|H_k\mathbf{y} - \beta\mathbf{e}_1\|_2, \end{aligned} \quad (4)$$

where $\beta = \|\mathbf{b}\|_2$ and \mathbf{e}_1 is the first vector of the normal basis of \mathbb{R}^{k+1} . A classical way to solve Equation (4) is to decompose the matrix H_k into QR using Givens rotations (Saad and Schultz, 1986) or Householder transformations (Walker, 1988), where Q is a $(k+1)$ -by- $(k+1)$ orthonormal matrix and R is a $(k+1)$ -by- k upper rectangular matrix. Then we have

$$\begin{aligned} \min_{\mathbf{y}} \|H_k\mathbf{y} - \beta\mathbf{e}_1\|_2 &= \min_{\mathbf{y}} \|QR\mathbf{y} - \beta\mathbf{e}_1\|_2 \\ &= \min_{\mathbf{y}} \|R\mathbf{y} - \mathbf{g}_{k+1}\|_2, \end{aligned} \quad (5)$$

where $\mathbf{g}_{k+1} = \beta Q^T \mathbf{e}_1$. Since the last row of R is zero, the solution of Equation (5) is obtained by solving an upper triangular system of linear equations which is a deflated matrix results from removing the last row of the matrix R and the last component of the vector \mathbf{g}_{k+1} .

Lemma 1.

Let the last row of H_k in Equation (4) be zero, i.e., $h_{k+1k} = 0$. Then $\mathbf{x} = V_k \mathbf{y}$ is the exact solution to $A\mathbf{x} = \mathbf{b}$.

Lemma 1 shows that for a consistent linear system of equations $A\mathbf{x} = \mathbf{b}$, the exact solution will be obtained in at most, after n steps. It is well known that the residual norms are monotonically decreasing with respect to k .

As the performance of GMRES method is expensive both in memory cost and complexity, one can often use its restarted version, so-called GMRES(k) method, in which the $K_k(A; \mathbf{r}_0)$ is restricted to be fixed dimension k and Arnoldi's process is confined using the latest iterate \mathbf{x}_k as a new initial approximation $\mathbf{x}_0 = \mathbf{x}_k$ for the restart. A good introduction to GMRES method may be found in the review article of Simoncini and Szyld (2007). Details on the theory and its implementation may be found in the article of Saad and Schultz (1986) and the monograph of Stoer and Bulirsch (2002). Recently, Bellalij et al. (2008) have established the equivalence of the approximation theory and the optimization approach to solving a min-max problem that arises in the convergence studies of the GMRES method and Arnoldi's process for normal matrices. Jiránek et al. (2008) analyzed the numerical behavior of several minimum residual methods, which are mathematically equivalent to the GMRES method. Gu (2005) and Gu et al. (2003) presented a variant of GMRES(k) augmented with some eigenvectors for the shifted systems. Niu et al. (2010) presented an accelerating strategy for weighted GMRES(k) (WGMRES(k)) method.

In addition, theoretical comparison of the Arnoldi's process and GMRES method, singular and nonsingular case of matrices, their breaks down and stagnation are discussed by Brown (1995) and Smoch (1999). Effort has been made to replace, by alternative methods, the rotations of Givens to improve speed, accuracy, and memory requirements of the GMRES method. Ayachour (2003) tried to reduce computational costs and storage requirements, but still needed to compute H_k^{-1} , in which H_k is formed by ignoring the first row of H_k .

In this paper, instead of QR factorization for solving the problem (4) a novel method based on the generalized Purcell (GP) method (Rahmani and Momeni-Masuleh, 2009) is presented. From a theoretical point of view, the proposed method is totally, different from Ayachour's method (2003). We analyze and compare the proposed method with GMRES(k) and WGMRES(k) methods with some challenges. The method has the luxury of not using Givens rotations unlike previous methods; it has no need to use orthogonal decomposition and moreover its computational costs are low. Especially when compared to Ayachour's method. The decomposition matrices of the Hessenberg matrix obtain from a simple and fast recursive relation.

The paper is organized as follows. In Section 2 the theoretical aspects of GP method is discussed. The Generalized Purcell minimal residual (GPMRES) method and the weighted GPMRES (WGPMRES) method are introduced. The theoretical analyses and the computational complexity are presented in Section 3. Section 4 provides four examples of standard sparse ill-conditioned matrices that are solved by the proposed method. In Section 5, we draw conclusions and give directions for future work.

2. GP Method for Minimal Residual

In this section, we explain the *GP* method that gives a unique decomposition of a given n -by- n matrix D into matrices R and F , in which R is a lower triangular matrix and F is a nonsingular matrix. Let \mathbf{d}_i^T , for $i = 1, 2, \dots, n$, denote the i -th row vector of matrix D and define

$$E^1 = \mathbf{e}_1^1, \mathbf{e}_2^1, \dots, \mathbf{e}_n^1,$$

where \mathbf{e}_i^1 is the i -th standard basis in \mathbb{R}^n . We construct a sequence of matrices E^j , each of which is a basis for \mathbb{R}^n , from the matrix E^{j-1} using matrix D . In the step j , suppose that we have

$$E^j = (\mathbf{e}_1^j, \mathbf{e}_2^j, \dots, \mathbf{e}_j^j, \mathbf{e}_{j+1}^j, \dots, \mathbf{e}_n^j).$$

To obtain the matrix E^{j+1} , the vectors \mathbf{e}_k^{j+1} for $k = j+1, \dots, n$ are constructed from a linear combination of \mathbf{e}_j^j and \mathbf{e}_k^j such that \mathbf{d}_j will be orthogonal to the $\mathbf{e}_{j+1}^{j+1}, \mathbf{e}_{j+2}^{j+1}, \dots, \mathbf{e}_n^{j+1}$ of E^{j+1} . To do this, we define

$$\mathbf{e}_k^{j+1} = \mathbf{e}_k^j - \alpha_{kj} \mathbf{e}_j^j, \quad k = j+1, \dots, n, \quad (6)$$

where

$$\alpha_{kj} = \frac{(\mathbf{e}_k^j, \mathbf{d}_j)}{(\mathbf{e}_j^j, \mathbf{d}_j)}, \quad (7)$$

resulting in a compact form

$$E^{j+1} = E^j - \mathbf{e}_j^j \begin{bmatrix} 0, \dots, 0, \alpha_{j+1j}, \dots, \alpha_{nj} \end{bmatrix}. \quad (8)$$

It is clear that the matrix $R = DE^n$ is a lower triangular matrix. Note that the matrix E^n is an upper triangular matrix whose all-diagonal entries are equal to 1 which implies that E^n is invertible. By setting F to the inverse of E^n , the decomposition process is complete.

Benzi and Meyer (1995) derived the same results up to this point. Now, we present the characteristics of matrices R and F .

Lemma 2.

The vector \mathbf{d}_j is linearly dependent on vectors \mathbf{d}_k $\prod_{k=1}^{j-1}$ if, for $i = j, \dots, n$, we have: $\mathbf{e}_i^j, \mathbf{d}_j = 0$.

Proof:

Regarding the decomposition process of D we have

$$\mathbb{R}^n = \text{Span } \mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_{j-1} \cup \text{Span } \mathbf{e}_j^j, \dots, \mathbf{e}_n^j. \tag{9}$$

Since $\mathbf{d}_j \in \mathbb{R}^n$ and by hypothesis $\mathbf{e}_i^j, \mathbf{d}_j = 0$, for $i = j, \dots, n$, so $\mathbf{d}_j \in \text{Span}\{\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_{j-1}\}$ which completes the proof.

Lemma 2 shows that we can find linearly dependent vectors and that the (j, j) th element of matrix R is zero. In this case we set apart \mathbf{d}_j , set $E^{j+1} = E^j$ and continue the process to \mathbf{d}_{j+1} . Therefore, there will be no a failed state in the process of GP method.

Theorem3.

For $k = 1, \dots, n$, every vector in \mathbb{R}^k can be expressed as a unique linear combination of vectors in E^k , i.e., E^k is a basis for \mathbb{R}^n .

Proof:

The proof is by induction on k . The statement is true for $k = 1$. Let the vectors of E^{k+1} be linearly dependent. It means that \mathbf{e}_i^i $\prod_{i=1}^k \cup \mathbf{e}_i^{k+1}$ $\prod_{i=k+1}^n$ are linearly dependent. Therefore, for some nonzero scalars γ_i , we have $\prod_{i=1}^k \gamma_i \mathbf{e}_i^i + \prod_{i=k+1}^n \gamma_i \mathbf{e}_i^{k+1} = 0$. Thanks to (6) we have

$$\prod_{i=1}^k \gamma'_i \mathbf{e}_i^i + \prod_{i=k+1}^n \gamma'_i \mathbf{e}_i^k = 0, \tag{10}$$

where $\gamma'_i = \gamma_i$ for $i \neq k$ and $\gamma'_k = \gamma_k - \prod_{i=k+1}^n \gamma_i \alpha_{ik}$. Using the induction hypothesis gives $\gamma_1 = \gamma_2 = \dots = \gamma_n = 0$, which is a contradiction.

Corollary 4.

Every E^j , for $j = 1, \dots, n$ is invertible.

To avoid dividing by zero in relation (7), we may select column vector \mathbf{d}_j such that

$$j = \text{argmax}_{j \leq k \leq n} |(\mathbf{d}_k, \mathbf{e}_j^j)|, \tag{11}$$

or column vector \mathbf{e}_j^j such that

$$j = \operatorname{argmax}_{j \leq k \leq n} |(\mathbf{d}_j, \mathbf{e}_k^j)|. \quad (12)$$

The operations (11) and (12) are called row pivoting and column pivoting, respectively.

Theorem 5.

In the case of the row pivoting method, suppose that \mathbf{e}_i^i be the computational value of \mathbf{e}_i^i , ϵ be a least upper bound of the computation error for α_{ij} , $\delta_{\mathbf{e}_n^n}$ be the relative computation error of \mathbf{e}_n^n and $\gamma = \max_{1 \leq i < n} \frac{\mathbf{e}_i^i}{\mathbf{e}_n^n}$. Then $\delta_{\mathbf{e}_n^n}$ is less than or equal to $\frac{\gamma\epsilon}{(1-\epsilon)}$.

Proof:

By the theorem hypothesis and relation (7) we have

$$|\alpha_{ij}| = \frac{d_j \mathbf{e}_i^j}{d_j \mathbf{e}_j^j} < \infty.$$

Let $\alpha_{ij} = \alpha_{ij} + \epsilon_{ij}$, for all i, j . Then

$$\begin{aligned} \mathbf{e}_n^n &= \mathbf{e}_n^{n-1} - \alpha_{n-1, n-1} \mathbf{e}_{n-1}^{n-1} \\ &= \mathbf{e}_n^{n-1} - (\alpha_{n-1, n-1} + \epsilon_{n-1, n-1}) \mathbf{e}_{n-1}^{n-1} \\ &= \mathbf{e}_n^{n-1} - \alpha_{n-1, n-1} \mathbf{e}_{n-1}^{n-1} - \epsilon_{n-1, n-1} \mathbf{e}_{n-1}^{n-1} \\ &= \mathbf{e}_n^n - \epsilon_{n-1, n-1} \mathbf{e}_{n-1}^{n-1}. \end{aligned}$$

Therefore, the vector \mathbf{e}_n^n must satisfy the recurrence

$$\mathbf{e}_n^n = \mathbf{e}_n^n - \epsilon_{n-1, n-1} \mathbf{e}_{n-1}^{n-1} + \epsilon_{n-1, n-1} \epsilon_{n-2, n-2} \mathbf{e}_{n-2}^{n-2} - \dots$$

and as a result

$$\mathbf{e}_n^n - \mathbf{e}_n^n = \sum_{i=1}^{n-1} (-1)^i \prod_{j=1}^i \epsilon_{n-j, n-j} \mathbf{e}_{n-i}^{n-i},$$

or

$$\delta_{\mathbf{e}_n^n} \approx \frac{\mathbf{e}_n^n - \mathbf{e}_n^n}{\mathbf{e}_n^n} \leq \gamma \sum_{i=1}^{n-1} \epsilon^i \leq \gamma \epsilon \sum_{i=0}^{\infty} \epsilon^i = \frac{\gamma\epsilon}{1-\epsilon}.$$

Lemma 6.

The complexity of Purcell method is $O(\frac{n^3}{3})$ (Rahmani, and Momeni-Masuleh, 2009).

Lemma 6 gives an upper bound for the computational complexity. As one can see in the next section, the nature of H_k and optimized operations allow us to have a low computational complexity (less than that given in Lemma 6).

3. GPMRES and WGPMRES Methods

In this section, we intend to propose the GPMRES method based on previous section for solving the least squares problem (4).

Let matrix H_k^T be the transpose of Hessenberg matrix H_k , which is produced by Arnoldi's process. Here H_k^T has the following form

$$H_k^T = \begin{pmatrix} h_{11} & h_{21} & 0 & \cdots & 0 \\ h_{12} & h_{22} & h_{32} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ h_{1\ k-1} & h_{2\ k-1} & h_{3\ k-1} & \cdots & 0 \\ h_{1k} & h_{2k} & h_{3k} & \cdots & h_{k+1\ k} \end{pmatrix} .$$

We decompose the matrix H_k^T in to $R, \mathbf{0} E^{-1}$ using the GP method, where the matrix R is a k -by- k lower triangular matrix and E is a $k + 1$ -by- $k + 1$ matrix. By Theorem 3, E is nonsingular and its columns span \mathbb{R}^{k+1} .

Decomposition is accomplished in k steps, in which we rectify $\mathbf{e}_i^1, i = 1, \dots, k + 1$ such that

$$H_k^T E = (R, \mathbf{0}). \tag{13}$$

Step 1: Suppose that E^l is given and has the following form

$$E^l = \mathbf{e}_2^1, \dots, \mathbf{e}_l^1, \mathbf{e}_1^l, \mathbf{e}_{l+1}^1, \dots, \mathbf{e}_{k+1}^1 ,$$

and that $h_{l+1\ l} \neq 0$. To have a simple form of H_k^T, \mathbf{e}_1^l is swapped by \mathbf{e}_{l+1}^1 . Using the GP method gives

$$\mathbf{e}_1^{l+1} = \mathbf{e}_1^l - \alpha_{1l} \mathbf{e}_{l+1}^1, \tag{14}$$

where

$$\alpha_{1l} = \frac{\mathbf{h}_{l+1}, \mathbf{e}_1^l}{(\mathbf{h}_{l+1}, \mathbf{e}_{l+1}^1)} = \frac{(\mathbf{h}_{l+1}, \mathbf{e}_1^l)}{h_{l+1\ l}} \tag{15}$$

in which \mathbf{h}_i^T is the i -th row vector of H_k^T . Since $h_{l+1}, \mathbf{e}_j^{l+1} = 0$, for $j = l + 2, \dots, k + 1$, the coefficients α_{jl} are all zero and therefore $\mathbf{e}_j^{l+1} = \mathbf{e}_j^l = \mathbf{e}_j^1$, which implies that

$$E^{l+1} = \mathbf{e}_2^1, \dots, \mathbf{e}_{l+1}^1, \mathbf{e}_1^{l+1}, \mathbf{e}_{l+2}^1, \dots, \mathbf{e}_{k+1}^1 .$$

Finally, at step k one can get

$$E = E^{k+1} = (\mathbf{e}_2^1, \dots, \mathbf{e}_{k+1}^1, \mathbf{e}_1^{k+1}), \quad (16)$$

where E is in the form of a $k + 1$ -by- $k + 1$ companion matrix. Note that by expanding the matrix E along the first row, we have $\det E = -1^{k+1}$ which implies that E is invertible.

As a result, according to the decomposition we get

$$\begin{aligned} e_{11}^{k+1} &= 1, \\ e_{i1}^{k+1} &= -\frac{\prod_{j=1}^{i-1} h_j e_{j1}^{k+1}}{h_{i-1}}, \quad i = 2, \dots, k + 1. \end{aligned} \quad (17)$$

Remark 1.

It is easy to see that

$$R = (\mathbf{h}_2, \mathbf{h}_3, \dots, \mathbf{h}_{k+1}). \quad (18)$$

Regarding to (13), we have

$$H_k = E^{-T} (R, \mathbf{0})^T,$$

where $E^{-T} = E^{-1 T}$. Now we have

$$\begin{aligned} \min_{\mathbf{y}} H_k \mathbf{y} - \beta \mathbf{e}_{1 \ 2} &= \min_{\mathbf{y}} E^{-T} (R, \mathbf{0})^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2} \\ &\leq E^{-T} \min_{\mathbf{y}} (R, \mathbf{0})^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2}. \end{aligned} \quad (19)$$

Theorem 7.

Suppose that E and R are given by (16) and (18), respectively. Then,

$$\operatorname{argmin}_{\mathbf{y}} (R, \mathbf{0})^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2} = 0,$$

and for $\mathbf{y} = \mathbf{0}$ we have

$$(R, \mathbf{0})^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2} = \beta.$$

Proof:

For a nonsingular matrix R and for every $\mathbf{y} \neq \mathbf{0}$ we get $R^T \mathbf{y} \neq \mathbf{0}$. Since $E^T \mathbf{e}_1 = \mathbf{e}_{k+1}$, we have

$$\forall \mathbf{y} \neq \mathbf{0}: \quad R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2} = \begin{matrix} R^T \mathbf{y} \\ \beta \end{matrix} > \beta,$$

for $\mathbf{y} = \mathbf{0}$ the proof is straightforward.

Theorem 7 leads to the trivial minimal residual solution $\mathbf{y} = \mathbf{0}$. In order to avoid this case, here we will give a non-trivial minimal residual solution with a lower bound less than β . At first we normalize \mathbf{e}_1^{k+1} and denote it by $\mathbf{e}_1^{k+1} = \omega_1, \omega_2, \dots, \omega_{k+1}^T$, where

$$\begin{aligned} \omega_1 &= \frac{1}{1 + \sum_{j=2}^{k+1} e_{j1}^{k+1 \ 2}}, \\ \omega_i &= \frac{e_{i1}^{k+1}}{1 + \sum_{j=2}^{k+1} e_{j1}^{k+1 \ 2}} \quad i = 2, 3, \dots, k + 1. \end{aligned} \tag{20}$$

Then, the vectors $\mathbf{e}_2^1, \mathbf{e}_3^1, \dots, \mathbf{e}_{k+1}^1$, using GP method, generate the vectors $\mathbf{e}_2^2, \mathbf{e}_3^2, \dots, \mathbf{e}_{k+1}^2$, which are perpendicular to \mathbf{e}_1^{k+1} .

Setting $E = (\mathbf{e}_2^2, \mathbf{e}_3^2, \dots, \mathbf{e}_{k+1}^2, \mathbf{e}_1^{k+1})$, it is easy to show that $E = EB$, where

$$B = \begin{matrix} I_k & \mathbf{0} \\ -\boldsymbol{\theta}_k^T & 1 \end{matrix} \quad \text{and} \quad E = \begin{matrix} \mathbf{0}^T & \omega_1 \\ I_k & \boldsymbol{\theta}_k \end{matrix},$$

in which $\boldsymbol{\theta}_k = \omega_2, \dots, \omega_{k+1}^T$. In other words,

$$E = \begin{matrix} -\omega_1 \boldsymbol{\theta}_k^T & \omega_1 \\ I_k - \boldsymbol{\theta}_k \boldsymbol{\theta}_k^T & \boldsymbol{\theta}_k \end{matrix}. \tag{21}$$

One can see that

$$B^{-1} = \begin{matrix} I_k & \mathbf{0} \\ \boldsymbol{\theta}_k^T & 1 \end{matrix} \quad \text{and} \quad E^{-1} = \begin{matrix} -\frac{\boldsymbol{\theta}_k}{\omega_1} & I_k \\ \frac{1}{\omega_1} & \mathbf{0}^T \end{matrix}.$$

Therefore,

$$E^{-1} = \begin{matrix} -\frac{\boldsymbol{\theta}_k}{\omega_1} & I_k \\ \omega_1 & \boldsymbol{\theta}_k^T \end{matrix},$$

and

$$\begin{aligned} H_k^T E &= H_k^T E B \\ &= R, \mathbf{0} B \\ &= R, \mathbf{0}. \end{aligned}$$

Then we have

$$H_k \mathbf{y} - \beta \mathbf{e}_{1-2} = E^{-T} R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1-2}. \quad (22)$$

Due to the definition of matrix B we know that $\|B^{-1}\|_2 = 1$, thus,

$$E^{-1} \leq E^{-1},$$

and

$$\min_{\mathbf{y}} H_k \mathbf{y} - \beta \mathbf{e}_{1-2} \leq E^{-T} \min_{\mathbf{y}} R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1-2}.$$

Since $\omega_1 > 0$, Gershgorin's theorem provides

$$E^{-1} \leq \rho E^{-T} E^{-1} = \frac{1}{1 - \omega_1^2},$$

which shows that the 2-norm of E^{-T} is bounded.

Theorem 8.

Suppose that, E and R are given by (21) and (18), respectively and R is nonsingular. Then,

$$\operatorname{argmin}_{\mathbf{y}} R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1-2} = -\beta \omega_1 R^{-T} \boldsymbol{\theta}_k,$$

and for $\mathbf{y} = -\beta \omega_1 R^{-T} \boldsymbol{\theta}_k$ we have

$$R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1-2} = \beta \omega_1.$$

Proof:

On account of

$$\begin{aligned} E^T \mathbf{e}_1 &= -\omega_1 \quad -\omega_2, \dots, -\omega_{k+1}, 1^T \\ &= \omega_1 \begin{matrix} -\boldsymbol{\theta}_k \\ 1 \end{matrix}, \end{aligned}$$

one can see that

$$\begin{aligned} \forall \mathbf{y}: \quad R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1-2} &= R^T \mathbf{y} + \beta \omega_k \boldsymbol{\theta}_k \frac{2}{2} + \beta^2 \omega_1^2 \\ &\geq \beta^2 \omega_1^2, \end{aligned}$$

as R is nonsingular, there exists a unique nonzero solution for $R^T \mathbf{y} = -\beta \omega_1 \boldsymbol{\theta}_k$ which minimize

$$R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2},$$

and the minimum at this case is equal to $\beta \omega_1 \leq \beta$.

Corollary 9.

Under the assumptions of Theorem 8, we have

$$\begin{aligned} \min_{\mathbf{y}} H_k \mathbf{y} - \beta \mathbf{e}_{1 \ 2} &\leq \rho \min_{\mathbf{y}} R, \mathbf{0}^T \mathbf{y} - \beta E^T \mathbf{e}_{1 \ 2} \\ &= \rho \beta \omega_1. \end{aligned}$$

Remark 2.

It is noticeable that GPMRES solution to the problem both in method and in results is different from that of GMRES method. Of course, if $E_2 = 1$ then GPMRES results are the same as GMRES, but still in this case, theoretically, the sequence of β_i is decreasing. When the E_2 is less than 1, GPMRES results are better than those of GMRES.

Hereafter, we will refer to the above process of finding \mathbf{y} as GPMRES method. We can use GPMRES method iteratively. The iterative version, termed by GPMRES(k), for solving $A\mathbf{x} = \mathbf{b}$ is summarized in Table 1.

Table 1: GPMRES(k) method

1.	Choose \mathbf{x}_0 .
2.	Compute $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$, $\beta = \ \mathbf{r}_0\ _2$ and let $\mathbf{v}_1 = \mathbf{r}_0 / \ \mathbf{r}_0\ _2$, Iterate: for $j = 1, 2, \dots, k$
	$h_{ij} = \frac{A\mathbf{v}_j, \mathbf{v}_i}{j} \quad i = 1, 2, \dots, j$
	$\mathbf{v}_{j+1} = A\mathbf{v}_j - \sum_{i=1}^j h_{ij} \mathbf{v}_i$
	$h_{j+1 \ j} = \ \mathbf{v}_{j+1}\ _2$
	$\mathbf{v}_{j+1} = \frac{\mathbf{v}_{j+1}}{h_{j+1 \ j}}$
3.	Construct \mathbf{e}_1^{k+1} and $\omega_i \quad i=1^{k+1}$ using Eqs. (17) and (20), respectively.
4.	Form the approximate solution: $\mathbf{y}_k = -\beta \omega_1 \ h_2, h_3, \dots, h_{k+1}^{-T} \boldsymbol{\theta}_k,$ $\mathbf{x}_k = \mathbf{x}_0 + V_k \mathbf{y}_k,$
	where $\boldsymbol{\theta}_k = -\omega_1, \dots, \omega_{k+1}^T$,
5.	If $\beta \omega_1 < \epsilon$ then stop, else define $\mathbf{x}_0 = \mathbf{x}_k$ and go to step 2.

3.1. GPMRES Properties

Theorem 10.

Let \mathbf{x}_0 be an initial guess. Define

$$\beta_0 = \|\mathbf{b} - A\mathbf{x}_0\|_2 = \|\mathbf{r}_0\|_2,$$

and

$$\beta_i = \|\mathbf{r}_{i-1} - A\mathbf{x}_i\|_2, \quad i = 1, 2, \dots,$$

where \mathbf{x}_i is the approximate solution obtained from the i th step of the GPMRES method. Then,

$$\beta_i < \beta_{i-1}, \quad i = 1, 2, \dots.$$

In addition, equality can happen only if $\beta_i = 0$ or $\mathbf{e}_1^{k+1} = \mathbf{e}_1$.

Proof:

It can be shown that

$$E^{-T} \mathbf{e}_{k+1}^1 = \begin{matrix} \omega_1 \\ \boldsymbol{\theta}_k \end{matrix}.$$

Substituting $\mathbf{y} = -\beta_0 \omega_1 R^{-T} \boldsymbol{\theta}_k$ in (22), leads to

$$\begin{aligned} \beta_1 &= \|E^{-T} R \mathbf{0}^T \mathbf{y} - \beta_0 E^T \mathbf{e}_1\|_2 \\ &= \|\beta_0 \omega_1 E^{-T} \mathbf{e}_{k+1}^1\|_2 \\ &= \beta_0 \omega_1 \|\begin{matrix} \omega_1 \\ \boldsymbol{\theta}_k \end{matrix}\|_2 \\ &= \beta_0 \omega_1. \end{aligned} \tag{23}$$

Regarding Equation (20), if $\omega_1 < 1$ then $\beta_1 < \beta_0$. Otherwise $\beta_1 = \beta_0$ only if $\mathbf{e}_1^{k+1} = \mathbf{e}_1$. In addition, equality can happen if $\beta_0 = 0$.

By assuming $\omega_1 \neq 1$ and $\beta_i \neq 0$ for $i = 1, 2, \dots$, in the same manner, we have

$$\beta_{i+1} = \beta_i \omega_1 < \beta_i.$$

An important consequence of this theorem is that

$$\beta_0 > \beta_1 > \dots > \beta_i > \dots.$$

As a result, the stopping criteria of the GPMRES method can be chosen as $\beta_i < \epsilon$ or $\omega_1 = 1$. In the latter case, one can iterate GPMRES method to obtain the desired solution to the problem in

Equation (1). In some steps if $\omega_1 = 1$ is happened, it shows that we cannot go further and the approximate solution at that step is the best one with the GPMRES method.

Theorem 11.

Suppose that in step i of GPMRES method we have $\beta_{i-1} \neq 0$ and $\omega_1 = 1$. Then the stagnation of the residual norm of GPMRES method will occur for the linear system of Equation (1).

Proof:

By assumption, Equation (20) yields $\theta_k = 0$. The conclusion of the Theorem follows from Equation (23) and the proof is complete.

Furthermore, according to Equation (17) we get

$$h_{11} = h_{12} = \dots = h_{1k} = 0,$$

or

$$Av_j; v_1 = 0, j = 1, 2, \dots, k.$$

Hence,

$$\mathbf{b} \notin \text{Span}\{A\mathbf{b}, A^2\mathbf{b}, \dots, A^{k-1}\mathbf{b}\}.$$

Remark 3.

In GPMRES method, unlike Ayachour's method (Ayachour, 2003), in order to get the solution for the case of $h_{k+1k} = 0$, there is no for any treatment. This situation is explained in the next theorem.

Theorem 12.

In the case of $h_{k+1k} = 0$, GPMRES method easily reaches the exact solution $\mathbf{x}_k = \mathbf{x}_0 + V_k \mathbf{y}$.

Proof:

Suppose that $h_{k+1k} = 0$. Then, the vector h_k is orthogonal to the vector e_{k+1}^1 and there is no need to replace e_1^k by e_{k+1}^1 . Hence $E = E^k$ and obviously $H_k^T E = (R^*, \mathbf{0})$, where R^* is the same as R except for the entry R_{kk}^* , which is

$$R_{kk}^* = \sum_{j=1}^k h_{kj} e_{j1}^k.$$

Therefore,

$$E^T \mathbf{e}_1 = \mathbf{e}_k. \quad (24)$$

Now, let $\mathbf{y} = \beta R_k^{-T}$, where R_k^{-T} is the last column of R^{-T} . Then,

$$\|H_k \mathbf{y} - \beta \mathbf{e}_1\|_2 = \|R \mathbf{0}^T \mathbf{y} - \beta \mathbf{e}_k\|_2 = 0.$$

Thus, \mathbf{y} is the minimum solution to the problem (19) and $\mathbf{x}_k = \mathbf{x}_0 + V_k \mathbf{y}$ is the exact solution of $A\mathbf{x} = \mathbf{b}$.

3.2. WGMRES Method

Suppose that $D = \text{diag}(d_1, d_2, \dots, d_n)$ be an arbitrary diagonal matrix with $d_i > 0$, for $i = 1, \dots, n$. For any vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, the D-scalar product is defined as

$$(\mathbf{u}, \mathbf{v})_D = \mathbf{v}^T D \mathbf{u} = \sum_{i=1}^n d_i u_i v_i,$$

and the associated D-norm is given by

$$\|\mathbf{u}\|_D = \sqrt{\mathbf{u}, \mathbf{u}}_D.$$

The WGMRES method can be derived from a weighted Arnoldi's process (Essai, 1998). The only difference between GMRES and WGMRES is that using the D-norm instead of a 2-norm for computing the β and $h_{j+1,j}$. Similarly, the WGMRES method can be derived easily from GPMRES, in which the β and $h_{j+1,j}$ are computed using the D-norm.

3.3. Computational Complexity

In order to calculate the number of operations in GPMRES method, consider the

$$H_k^T = (\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_{k+1})$$

be the column-by-column representation of matrix H_k^T . As we know GPMRES method only requires to compute

$$E^T \mathbf{e}_1 = \omega_1 \begin{pmatrix} -\boldsymbol{\theta}_k \\ 1 \end{pmatrix}.$$

This is accomplished without explicit storage of E^T , by calculating the normalized vector \mathbf{e}_1^{k+1} and storage of $\boldsymbol{\theta}_k$ and ω_1 .

The computational cost in performance of the one step of GPMRES is $k^2 + 4k + 1$ multiplications, while in GMRES method by using Givens rotations the computational cost is $\frac{5k^2 + 13k}{2}$ multiplications while Ayachour's method (Ayachour, 2003) needs $k^2 + 6k$

multiplications. The cost of the GMRES method can vary significantly, if we use QR decomposition.

4. Numerical Results

In order to elucidate the theoretical results of the GPMRES (k) and WGMRES (k) methods four examples are presented. In all the examples, the initial vector x_0 is zero and the result of every inner iteration k is selected as initial vector for next inner iteration $k + 1$. To decompose H_k in GMRES(k) or WGMRES(k), instead of the Givens rotations, the standard QR decomposition algorithm from *MATLAB version 7* is used. All example matrices are obtained from the Matrix Market (Website, 2010) and computations, including GMRES(k) and WGMRES(k), are accomplished using our written MATLAB codes.

Example 1: Consider the linear system of equations $Ax = b$, in which A is the ill-conditioned matrix

$$\text{STEAM1}(\|A\|_2 = 2.2 \times 10^7, k(A) \approx 3 \times 10^7, n = 240)$$

and $b = A^{-1} \mathbf{1}$, $\mathbf{1} = [1, 1, \dots, 1]^T$. The normwise backward error $\frac{\|b - Ax_n\|_2}{\|A\|_2 \|x_n\|_2}$ for GPMRES(k), GMRES(k) and Ayachour's method, which is termed by GMRES-Aya are plotted in Figure 1. In comparison to the RB-SGMRES and GCR methods (Jiránek et al., 2008, Figure 3.5), the results show that the GPMRES(k), GMRES(k) and GMRES-Aya converge to the log of normwise backward error less than 10^{-16} at iteration number before $k = 80$, while the RB-SGMRES and GCR methods reach the same value at $k = 200$. Furthermore, GPMRES(k) gives more accurate approximate solution than the others.

Example 2: Consider the matrix

$$\text{FS1836}(\|A\|_2 \approx 1.2 \times 10^9, k(A) \approx 1.7 \times 10^{11}, n = 183)$$

and b is equal to the left singular vector corresponding to the smallest singular value of A . The backward error $\frac{\|b - Ax_n\|_2}{\|A\|_2 \|x_n\|_2 + \|b\|_2}$ for GPMRES(k), GMRES(k) and GMRES-Aya are shown in Figure 2. In comparison to the adaptive Simpler GMRES (Jiránek and Rozložník, 2010, Figure 5) results show that GPMRES(k) converges to the log of backward error less than 10^{-20} at iteration number $k = 22$, while the log of backward error of adaptive Simpler GMRES for iteration number $k = 60$ is at most 10^{-17} . Here, again GPMRES(k) method gives better results than the others.

Example 3: Consider the matrix *FS1836* and $b = A^{-1} \mathbf{1}$. The log of backward error for GPMRES(k), GMRES(k) and GMRES-Aya are presented in Figure 3. The results show that the log of backward error for GMRES-Aya and GMRES(k) are same as the log of backward error of the adaptive Simpler GMRES while GPMRES(k) method has less log of backward error than 10^{-20} . Also GMRES(k), GMRES-Aya and adaptive Simpler GMRES (Jiránek and Rozložník, 2010, Figure 3) cannot converge to less than 10^{-17} .

Example 4: In this example, we test the matrix *memplus* whose size is 17758 with 126150 non-zero entries. Here, WGMRES(k) is tested and compared with the WGMRES(k) (Niu, Lu, and Zhou, 2010) and the weighted GMRES-Aya (WGMRES-Aya) methods. The residual norm $(\frac{r_k}{\|b\|_2})$ for the WGMRES(k), WGMRES(k) and WGMRES-Aya methods are presented in Figure 4. The results show that the residual norm for the WGMRES-Aya and the WGMRES(k) are the same as the residual norm of WGMRES(k) up to nearly 30 iterations for $k = 15$, while the WGMRES(k) gives better residual norm for iteration number bigger than 45.

5. Conclusion

A new iterative method based on GP method for the solution of large, sparse, and non-symmetric systems of linear equations is proposed. The GPMRES(k) method does not need orthogonal decomposition of Hessenberg matrix. In comparison to some fast implementation methods for the GMRES like GMRES-Aya, the proposed method has smaller computational cost, easy implementation and no need to any further treatment for the case of $h_{k+1,k} = 0$. Also, the stagnation case can be identified by checking the ω_1 . The convergence of the method to minimal residual is obvious based on theoretical discussion and depends strongly on ω_1 which is less than 1. Our experiences show that the performance of GPMRES(k) method for solving ill-conditioned problems, is equivalent or even has lower residual norm error in comparison to the improved versions of GMRES method such as the Simpler GMRES, the adaptive version of the Simpler GMRES, the GMRES-Aya(k) and the WGMRES(k) methods or the WGMRES-Aya(k) method. Further work is needed to investigate the impact of ω_1 for accelerating convergence of the restarted GPMRES(k) method and improving the proposed method for augmented restarted WGMRES(k).

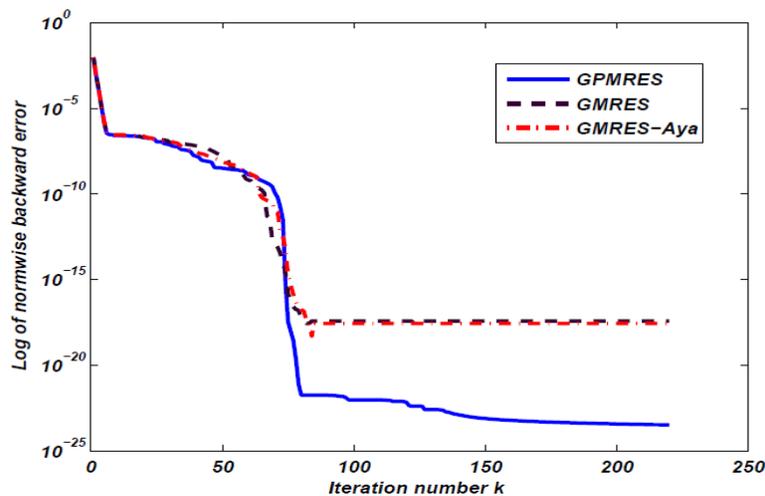


Figure 1. The log normwise backward error of $Ax = b$ solved by GPMRES (k), GMRES(k) and GMRES-Aya methods. A is STEAM1 matrix and $b = A [1, \dots, 1]^T$

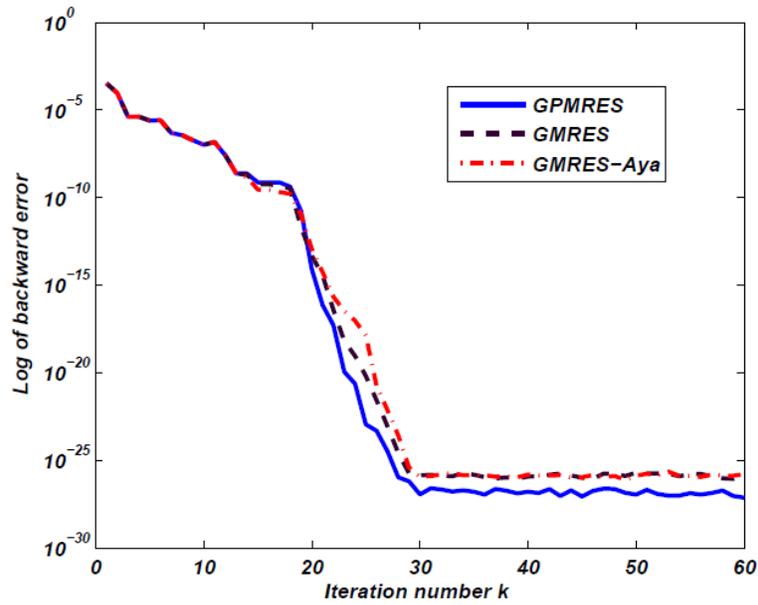


Figure 2. The log backward error for $Ax = b$ solved by GPMRES(k), GMRES(k) and GMRES-Aya methods. A is matrix FS1836 and b is the left singular vector corresponding to the smallest singular value of matrix A

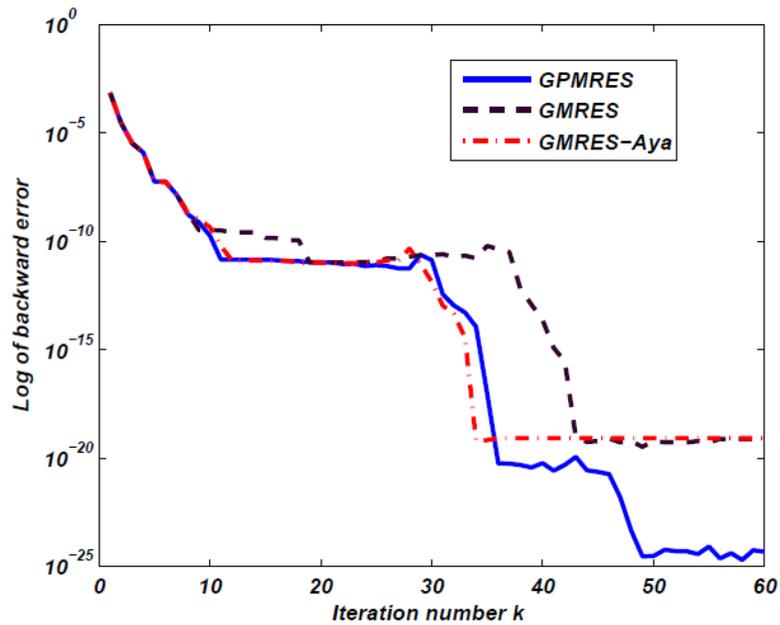


Figure 3. The log backward error of $Ax = b$ solved by GMRES(k), GMRES(k) and GMRES-Aya methods. A is matrix FS1836 and $b = A^{-1} \cdot \mathbf{1}^T$

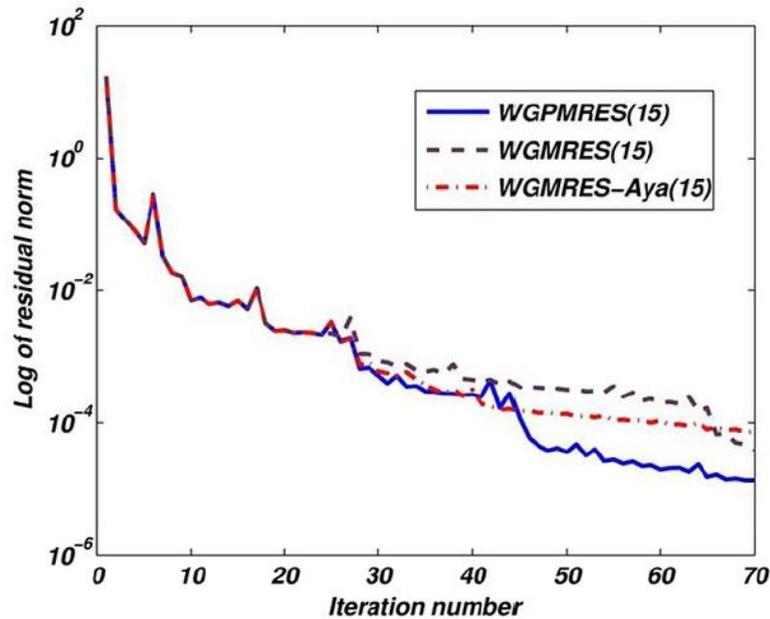


Figure 4. The log residual norm of $Ax = b$ solved by WGPMRES(15), WGMRES(15) and WGMRES-Aya(15) methods for the matrix memplus

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