Journal of Mathematical Modeling
Vol. 9, No. 3, 2021, pp. 239-256

JMM

Augmented and deflated CMRH method for solving nonsymmetric linear systems

Zohreh Ramezani, Faezeh Toutounian*
Department of Applied Mathematics, School of Mathematical Sciences, Ferdowsi University of Mashhad, Iran

Email(s): z_ramezani1367@yahoo.com,toutouni@math.um.ac.ir

Abstract. The CMRH (Changing Minimal Residual method based on the Hessenberg process) is an iterative method for solving nonsymmetric linear systems. The method generates a Krylov subspace in which an approximate solution is determined. The CMRH method is generally used with restarting to reduce the storage. Restarting often slows down the convergence. In this paper we present augmentation and deflation techniques for accelerating the convergence of the restarted CMRH method. Augmentation adds a subspace to the Krylov subspace, while deflation removes certain parts from the operator. Numerical experiments show that the new algorithms can be more efficient compared with the CMRH method.

Keywords: Krylov subspace methods, augmentation, deflation, CMRH method, GMRES method, harmonic Ritz values.
AMS Subject Classification 2010: 65F10.

1 Introduction

In this paper we consider the solution of the linear system of equations

$$Ax = b, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is a nonsingular matrix and $b \in \mathbb{R}^n$ is a given vector.

A popular class of iterative methods for solving system (1) is Krylov subspace methods. Krylov subspace methods find an approximate solution

$$x_m \in x_0 + \mathcal{K}_m(A, r_0), \tag{2}$$

where $\mathcal{K}_m(A, r_0) \equiv \mathrm{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$ denotes an m-dimensional Krylov subspace, x_0 is the initial guess and r_0 is the initial residual. GMRES is one of the most popular Krylov

*Corresponding author.
Received: 2 September 2020 / Revised: 18 October 2020 / Accepted: 22 October 2020
DOI: 10.22124/jmm.2020.17024.1511

subspace methods for solving system (1). Another method is Quasi-Minimal Residual method (QMR) which has low storage rather than GMRES. GMRES often exhibits steady convergence, while QMR convergence curves are characterized by plateaus and sudden drops.

In [36], CMRH method is presented for solving (1) similar to QMR, but uses another basis for the Krylov subspace. This basis is constructed by the Hessenberg process. This technique requires less arithmetic operations and storage than Arnoldi process because, at iteration k, it constructs a lower trapezoidal basis $l_1, l_2, \dots, l_k$, where l_i is a vector having $(i-1)$ leading zero components and one component is equal to one. Hence, for a dense matrix, performing the matrix-vector product Al_i is achieved with a lower cost comparing to Arnoldi process. Similarly to GMRES, this method requires one matrix-vector product per iteration. Heyouni and Sadok [24] proposed an implementation of the CMRH method which minimizes memory requirements. Some recent developments concerning the CMRH method and the Hessenberg process can be found in [1–3, 14, 20, 21, 25, 27, 37, 38, 40]. In [13], Duminil presented an implementation for parallel architectures and an implementation of the left-preconditioned CMRH method.

As GMRES, the CMRH method is often used with restarting strategy to reduce storage, but restarting slows the convergence of the methods and can make them stagnate in some situations.

Deflation and augmentation are two techniques for accelerating the convergence of Krylov subspace methods. In augmentation and deflation approaches, the search space of the method $\mathcal{K}_m$ is made larger by an appropriately selected subspace $\mathcal{U}$ in every step, or the Krylov subspace method is used for solving a projected problem and then a correction step is applied at the end. The first deflation and augmentation techniques for solving linear systems were presented by Nicolaides [32] and Dostàl [9]. For symmetric positive definite matrix A, Saad et al. [35] described a deflated version of the CG algorithm. Also, Vuik et al. [39] applied deflated CG with incomplete Cholesky preconditioning for the solution of a class of layered problems with extreme contrasts in the coefficients. For nonsymmetric systems Chapman and Saad [8] and Morgan [29–31] proposed augmentation of Krylov subspaces generated by restarted GMRES method by spaces spanned by certain eigenvectors or Ritz vectors. Convergence properties of Krylov subspace methods augmented by spaces close to invariant subspaces are discussed by Saad [34]. These deflation and augmention techniques are more suitable for some types of problems than others. They can be very effective when convergence is being hampered by a few eigenvalues [29]. However, they may have little effect on highly non-normal problems [8]. In [12, 18, 19], for some of well-known methods, it was shown that the convergence behavior of Krylov subspaces methods for non-normal matrices does not depend on the eigenvalues of the matrix only. In addition, it may be impossible to obtain useful eigenvalue approximations from either Ritz values [11] or harmonic Ritz values [10] during restart cycles. Baglama and Reichel [4] proposed to augment the Krylov subspace determined by GMRES by an arbitrary linear space of low dimension. Baker *et al.* [5] used the error approximation for augmenting the next approximation space. For an excellent overview of deflated Krylov subspace methods in the Hermitian and non-Hermitian cases, we refer the reader to [15–17, 22, 23], where extensive bibliographical references and historical comments can be found.

In this paper we present deflation and augmentation techniques that have been designed to accelerate the convergence of the CMRH(m) (restarting CMRH) method for the solution of linear systems of equations. We propose two strategy that allow augmentation of the Krylov subspaces generated by CMRH method by a space close to an invariant subspace of A. In addition, we introduce a deflated CMRH method that is analogous to deflated GMRES method [22], but replaces the Arnoldi process by the Hessenberg process. Approximate spectral information which is required to define the augmentation space is provided by the Hessenberg process. Also deflated CMRH can break down in the same way as deflated GMRES. We show that breakdowns cannot occur if the augmentation space is an exact A-invariant subspace.

The paper is organized as follows. In Section 2, we shortly review the Hessenberg process and CMRH method. We present two augmented CMRH methods in Section 3. In Section 4, we describe a combined deflated and augmented CMRH method and show that under certain conditions, the method determines a solution without breakdown. Section 5 demonstrates the effectiveness of the proposed methods. Conclusions are summarized in Section 6.

Throughout the paper, all vectors and matrices are assumed to be real. We denote the range (or, the image) of a matrix M by $\mathcal{R}(M)$. For the null space (or kernel) of M we write $\mathcal{N}(M)$. For a vector v, $\|v\|$ always denotes the Euclidean norm $\|v\| = \sqrt{(v^T v)}$ and $\|v\|_\infty$ denotes the maximum norm $\|v\|_\infty = \max_{i=1,\dots n} |v_i|$, where v_i is the ith component of the vector v. $Z^\dagger$ denotes the pseudo-inverse of the matrix Z; see, for example, [36]. Some MATLAB notation is used; for instance, $H_k(i+1:m+1, 1:m)$ denotes the portion of H_k with rows from $i+1$ to $m+1$ and columns from 1 to m. Finally, I_k is the $k \times k$ identity matrix. e_j and $e_j^{(s)}$ denote the jth column of identity matrices I_n and I_s, respectively. The symbol $\leftrightarrow$ means swapping contents: $x \leftrightarrow y \Leftrightarrow t = x; x = y; y = t$.

2 CMRH algorithm

The CMRH method is an algorithm for solving nonsymmetric linear systems in which the Arnoldi component of GMRES is replaced by the Hessenberg process (see [36]). Given an initial guess x_0 for the exact solution $x^\star = A^{-1}b$, the Hessenberg process with pivoting constructs a basis of the Krylov subspace $\mathcal{K}_m(A, r_0) = \mathrm{span}\{r_0, Ar_0, \dots, A^{m-1}r_0\}$, where $r_0 = b - Ax_0$ is the initial residual.

Let $l_1 = r_0/(r_0)_{p_1}$, where $p_1 \in \{1, \dots, n\}$ is such that $|(r_0)_{p_1}| = \| r_0 \|_\infty$. The Hessenberg process with pivoting computes a matrix $L_m = [l_1, \dots, l_m]$ whose columns form a basis of the Krylov subspace $\mathcal{K}_m(A, r_0)$ by using the formulas

$$w = Al_j - \sum_{i=1}^{j} h_{i,j} l_i, \quad \text{for} \quad j = 1, \dots, m,$$

and

$$h_{j+1,j} l_{j+1} = w.$$

The parameters $h_{i,j}$ are determined such that

$$l_{j+1} \perp e_{p_1}, \dots, e_{p_j} \quad \text{and} \quad (l_{j+1})_{p_{j+1}} = 1,$$

where $p_i \in \{1, 2, \dots, n\}$ and $p_{j+1} = i_0$, and i_0 satisfies $\|w\|_\infty = |(w)_{i_0}|$. Let $\bar{H}_j$ be the $(j+1) \times j$ upper Hessenberg matrix whose nonzero entries are the $h_{i,j}$, and let H_j be the matrix obtained from $\bar{H}_j$ by deleting its last row, we have

$$\begin{aligned} AL_j &= L_{j+1}\bar{H}_j \\ &= L_j H_j + h_{j+1,j} l_{j+1} (e_j^{(j)})^T. \end{aligned} \tag{3}$$

If p denotes the permutation vector defined by $p_1, p_2, \ldots, p_n$ (as in Algorithm 1) and

$$P_n = [e_{p_1}, e_{p_2}, \ldots, e_{p_n}]^T,$$

denotes the $n \times n$ permutation matrix defined by the vector p, then we can easily check that $P_n L_j$ is a unit lower trapezoidal matrix. Using (3), the jth iterates of CMRH is defined by

$$x_j = x_0 + L_j y_j,$$

where y_j minimizes the following problem:

$$\min_{y \in \mathbb{R}^j} \parallel \bar{H}_j y - (r_0)_{p_1} e_1^{(j+1)} \parallel .$$

So, the iterate x_j can be written as

$$x_j = x_0 + L_j \bar{H}_j^{\dagger} (r_0)_{p_1} e_1^{(j+1)}. \tag{4}$$

Notice that if $\|w\|_\infty = 0$ at step j, then, in exact arithmetic, the degree of the minimal polynomial of A with respect to the vector r_0 is j [26] and we have constructed an invariant subspace and the process must be stopped. In this case, x_j is the exact solution of (1), (see Theorem 3 of [36]). CMRH(m) algorithm can be summarized as shown in Algorithm 1. More details about the CMRH algorithm can be found in [36].

Finally, we recall the definition of a harmonic Ritz pair [33] which is required to define the augmentation space.

Definition 1. Consider a subspace $\mathcal{W}$ of $\mathbb{C}^n$. Given a matrix $A \in \mathbb{C}^{n \times n}, \tilde{\theta} \in \mathbb{C}$, and $\tilde{y} \in \mathcal{W}$, $(\tilde{\theta}, \tilde{y})$ is a harmonic Ritz pair of A with respect to $\mathcal{W}$ if and only if

$$A\tilde{y} - \tilde{\theta}\tilde{y} \perp A\mathcal{W},$$

or equivalently, for the canonical scalar product,

$$\forall \tilde{w} \in \mathcal{R}(A\mathcal{W}), \qquad \tilde{w}^H (A\tilde{y} - \tilde{\theta}\tilde{y}) = 0.$$

We call $\tilde{y}$ a harmonic Ritz vector associated with the harmonic Ritz value $\tilde{\theta}$.

Assume that the columns of $W_s = [w_1, w_2, \ldots, w_s] \in \mathbb{R}^{n \times s}$ constitute a basis of $\mathcal{W}$, the harmonic Ritz pairs $(\tilde{\theta}_i, \tilde{y}_i), i = 1, 2, \ldots, s$, can be obtained by solving the small generalized eigenvalue problem

$$W_s^T A^T A W_s g_i = \tilde{\theta}_i W_s^T A^T W_s g_i, \qquad \tilde{y}_i = W_s g_i, \qquad i = 1, 2, \ldots, s. \tag{5}$$

Algorithm 1. CMRH(m) method

Choose m.
Start: for given x_0, *compute* $r_0 = b - Ax_0$ *and set* $p = [1, 2, \ldots, n]^T$.
Determine i_0 *such that* $|(r_0)_{i_0}| = \|r_0\|_\infty$, $l_1 = r_0/(r_0)_{i_0}$, $p_1 \leftrightarrow p_{i_0}$
Iterate: For $j = 1, \ldots, m$
  $u = Al_j$,
  For $i = 1, \ldots, j$
    $h_{i,j} = (u)_{p_i}$,
    $u = u - h_{i,j} l_i$,
  end
  If ($j < n$ *and* $u \neq 0$) *then*
    Determine $i_0 \in \{j+1, \ldots, n\}$ *such that* $|(u)_{p_{i_0}}| = \|(u)_{p_{j+1}:p_n}\|_\infty$,
    $h_{j+1,j} = (u)_{p_{i_0}}$, $l_{j+1} = u/h_{j+1,j}$, $p_{j+1} \leftrightarrow p_{i_0}$
  else
    $h_{j+1,j} = 0$, *Stop.*
  end
  If (an estimate of) $\| b - Ax_j \|$ *is small enough or* $j = n$ *then*
    $x_j = x_0 + [l_1, \ldots, l_j] * y_j$, *where* y_j *minimizes* $\| \bar{H}_j y - (r_0)_{p_1} e_1^{(j+1)} \|, y \in \mathbb{R}^j$.
      Stop iteration
  end
end
  $x_m = x_0 + [l_1, \ldots, l_m] * y_m$, *where* y_m *minimizes* $\| \bar{H}_m y - (r_0)_{p_1} e_1^{(m+1)} \|$, $y \in \mathbb{R}^m$.
  $x_0 := x_m$, *go to Start.*

3 Adding approximate eigenvector to the subspace

Restarting CMRH may lead to poor convergence and even stagnation. The convergence can be improved in many situations. For accelerating the convergence of restarting CMRH, as restarting GMRES [28, 29, 31], we propose that approximate eigenvectors corresponding to a few of the smallest eigenvalues in magnitude be formed and added to the Krylov subspace for CMRH. We present two implementations of the augmented CMRH method. In the implementations presented here, the subspace of projection is of the form $\mathcal{K} = \mathcal{K}_m + \mathcal{U}_k$, where $\mathcal{K}_m$ is the standard Krylov subspace whose dimension is m and $\mathcal{U}_k = \text{span}\{U_k\}$ is a subspace with dimension k, where $U_k = [\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k]$ with $\tilde{y}_i$, $i = 1, \ldots, k$, being the harmonic Ritz vectors corresponding to the k smallest harmonic Ritz values (in magnitude).

Let $s = m + k$. In the first algorithm (called augmented-CMRH algorithm), the solution space $\mathcal{K}$ is defined by

$$\mathcal{K} = \text{span}\{\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k, l_{k+1}, l_{k+2}, \ldots, l_s\},$$

where $l_{k+1}, l_{k+2}, \ldots, l_s$ are the Hessenberg vectors. Let $W_s = [\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k, l_{k+1}, l_{k+2}, \ldots, l_s]$ be the $n \times s$ matrix whose columns are basis vectors for the augmented subspace $\mathcal{K}$. We first compute the LU factorization with pivoting

$$AU_k = L_k R_k, \tag{6}$$

where $R_k \in \mathbb{R}^{k\times k}$ is upper triangular and $L_k \in \mathbb{R}^{n\times k}$. Let $p = [p_1, p_2, \ldots, p_n]^T$ be the permutation vector and $P_n = [e_{p_1}, e_{p_2}, \ldots, e_{p_n}]^T$ be the permutation matrix defined by this LU factorization with pivoting, so, $\hat{L}_k = P_n L_k$ is the lower trapezoidal matrix.

Letting $P_k = [e_{p_1}, e_{p_2}, \ldots, e_{p_k}]^T$ and using the oblique projector $Q = L_k(P_k L_k)^{-1}P_k$ on the subspace generated by the basis $L_k = [l_1, l_2, \ldots, l_k]$, and along the subspace generated by the basis $P_k^T = [e_{p_1}, e_{p_2}, \ldots, e_{p_k}]$, we define the normalized vector

$$l_{k+1} = \frac{(I - L_k C_n)r_0}{((I - L_k C_n)r_0)_{\tilde{p}_{k+1}}}, \tag{7}$$

where $C_n = (P_k L_k)^{-1}P_k$, r_0 is the residual vector from previous cycle, $\tilde{p}_{k+1} = i_0$, and i_0 satisfies $\|(I - L_k C_n)r_0\|_\infty = |((I - L_k C_n)r_0)_{i_0}|$. Using $\tilde{p}_{k+1}$, we update the permutation vector p. We then append columns to L_k, which are determined by a modified Hessenberg process with pivoting. The initial vector for the modified Hessenberg process is chosen to be l_{k+1}. The generated vectors are appended to the matrix L_k as they become available. After m steps of this modified Hessenberg process with pivoting, we have

$$AW_s = L_{s+1}\bar{H}_s, \tag{8}$$

where $L_{s+1} = [L_k \quad l_{k+1}, \ldots, l_{s+1}] \in \mathbb{R}^{n\times(s+1)}$.

Let $\tilde{p} = [p_1, \ldots, p_k, \tilde{p}_{k+1}, \ldots, \tilde{p}_n]^T$ denotes the updated permutation vector p and $\tilde{P}_n = [e_{p_1}, \ldots, e_{p_k}, e_{\tilde{p}_{k+1}} \ldots, e_{\tilde{p}_n}]^T$ denotes the updated permutation matrix P_n obtained after m steps of the modified Hessenberg process with pivoting, then $\hat{L}_{s+1} = \tilde{P}_n L_{s+1}$ is a lower trapezoidal matrix. We mention that the first column of trailing $n\times(m+1)$ submatrix $L_{s+1}(:, k+1 : s+1)$ of L_{s+1} is l_{k+1} defined by (7) and remaining columns of $L_{s+1}(:, k+1 : s+1)$ are determined by the m steps of the modified Hessenberg process. The leading principal $k\times k$ submatrix of the upper Hessenberg matrix $\bar{H}_s \in \mathbb{R}^{(s+1)\times s}$ is the upper triangular matrix R_k in the LU factorization (6). The entries of the trailing m columns of $\bar{H}_s$ are determined by the modified Hessenberg process. In addition, by defining the vector $f_{s+1} = [\gamma_1, \ldots, \gamma_k, \gamma_{k+1}, 0, \ldots, 0]^T \in \mathbb{R}^{s+1}$, where $[\gamma_1, \ldots, \gamma_k]^T = C_n r_0$ and $\gamma_{k+1} = ((I - L_k C_n)r_0)_{\tilde{p}_{k+1}}$, we can easily show that $r_0 = L_{s+1}f_{s+1}$. The sth iterate of augmented CMRH is defined by

$$x_s = x_0 + W_s d, \tag{9}$$

where $d \in \mathbb{R}^s$. From the relation (8) and the definition of vector f_{s+1}, we have

$$r_s = b - Ax_s = r_0 - AW_s d = L_{s+1}(f_{s+1} - \bar{H}_s d).$$

Since L_{s+1} is not orthogonal, as CMRH method, we obtain d such that $\| f_{s+1} - \bar{H}_s d \|$ is minimized. Hence (9) can be written as

$$x_s = x_0 + W_s \bar{H}_s^\dagger f_{s+1}.$$

To find approximate eigenvectors of A, using the subspace spanned by the columns of W_s, the relation (5), and $AW_s = L_{s+1}\bar{H}_s$, we solve the small generalized eigenvalue problem

$$\bar{H}_s^T L_{s+1}^T L_{s+1}\bar{H}_s g_i = \tilde{\theta}_i \bar{H}_s^T L_{s+1}^T W_s g_i. \tag{10}$$

The g_i's associated with the k smallest harmonic Ritz values (in magnitude) $\tilde{\theta}_i$ are needed and the corresponding harmonic Ritz vectors $\tilde{y}_i = W_s g_i, i = 1, \ldots, k$, will be used for adding to the next Krylov subspace. If $\tilde{y}_i$ is complex, the real and imaginary parts are used separately.

We mention that, the implementation is a little different for the first cycle ($i = 0$). Standard CMRH(s) is used and $W_s = L_s$ is produced with the Hessenberg process by the initial vector r_0. The algorithm is given just for the second and subsequent runs.

Now we can summarize one restart cycle i of augmented-CMRH algorithm as shown in Algorithm 2.

Algorithm 2. One restart cycle i of the augmented-CMRH(m,k)

Let $\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k$ be given harmonic Ritz vectors.
Compute $r_i = b - Ax_i$ and $s = m + k$. Set $w_j = \tilde{y}_j$, for $j = 1, \ldots, k$ and $p = [1, 2, \ldots, n]^T$.
Perform the LU factorization of $AW_s(:, 1 : k)$ as $AW_s(:, 1 : k) = L_k U_k$ with the permutation matrix $P_k^T = [e_{p_1}, e_{p_2}, \ldots, e_{p_n}]$.
Set $L_{s+1}(1 : n, 1 : k) = L_k$ and $H(1 : k, 1 : k) = U_k$,
Set $u = r_i$
For $j = 1, \ldots, k$
  $\gamma_j = (u)_{p_j}, \quad u = u - \gamma_j l_j$
end
Determine $i_0 \in \{k + 1, \ldots, n\}$ such that $|(u)_{p_{i_0}}| = \|(u)_{p_{k+1}:p_n}\|_\infty$, set $\gamma_{k+1} = (u)_{p_{i_0}}$ and $p_{k+1} \leftrightarrow p_{i_0}$.
Set $l_{k+1} = u/\gamma_{k+1}$,
For $j = k + 1, \ldots, s$
  $u = Al_j$,
  For $t = 1, \ldots, j$
    $h_{t,j} = (u)_{p_t}, \quad u = u - h_{t,j} l_t$,
  end
  If ($u \neq 0$) then
    Determine $i_0 \in \{j+1, \ldots, n\}$ such that $|(u)_{p_{i_0}}| = \|(u)_{p_{j+1}:p_n}\|_\infty$, $h_{j+1,j} = (u)_{p_{i_0}}$, $l_{j+1} = u/h_{j+1,j}$, $p_{j+1} \leftrightarrow p_{i_0}$.
  else
    $h_{j+1,j} = 0$, *Stop.*
  end
  Set $w_j = l_j$.
end
Set $L_{s+1} = [l_1, l_2, \ldots, l_{s+1}]$, $W_s = [w_1, w_2 \ldots, w_s]$, $\bar{H}_s = \{h_{i,j}\}_{1 \leq i \leq j+1; 1 \leq j \leq s}$
Set $f_{s+1} = [\gamma_1, \ldots, \gamma_k, \gamma_{k+1}, 0, \ldots, 0]^T \in \mathbb{R}^{s+1}$.
Compute $x_{i+1} = x_i + W_s \hat{d}$, where $\hat{d}$ minimizes $\| f_{s+1} - \bar{H}_s d \|$, $d \in \mathbb{R}^s$.
Solve the generalized eigen problem $\bar{H}_s^T L_{s+1}^T L_{s+1} \bar{H}_s g_j = \tilde{\theta}_j \bar{H}_s^T L_{s+1}^T W_s g_j$ for the appropriate g_j and form $\tilde{y}_j = W_s g_j$ for $j = 1, 2, \ldots, k$.

In the implementation of second algorithm (called CMRH-E), as GMRES-E [29], we first generate the basis of the Krylov subspace $\mathcal{K}_m$, then we add the approximate eigenvectors to it. Suppose that $[l_1, l_2, \ldots, l_m]$ have been produced by Hessenberg process (with pivoting) with initial vector r_0, and k harmonic Ritz vectors have been derived from the previous cycle. Let $W_s = [l_1, l_2, \ldots, l_m, \tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k]$, a slight modification in the Hessenberg procedure is used to deduce a trapezoidal basis of $\mathcal{K}$. It consists of defining u in Algorithm 1 (line 5 of Algorithm 1) now as

$$u = Al_j \qquad (1 \leq j \leq m) \qquad \text{and} \qquad u = A\tilde{y}_{j-m} \qquad (m+1 \leq j \leq s).$$

With this definition, we obtain the modified Hessenberg relation $AW_s = L_{s+1}\bar{H}_s$, where $L_{s+1} = [l_1, l_2, \ldots, l_{s+1}]$ is an $n \times (s+1)$ matrix and $\bar{H}_s$ is an $(s+1) \times s$ upper-Hessenberg matrix. Let $P_{s+1} = [e_{p_1}, e_{p_2}, \ldots, e_{p_n}]^T$ denotes the permutation matrix obtained after s steps of the modified Hessenberg process, then $\hat{L}_{s+1} = P_{s+1}L_{s+1}$ is a lower trapezoidal matrix.

The approximate solution of system (1) can be written as $x_s = x_0 + W_s d$, where $d \in \mathbb{R}^s$. So, we have

$$r_s = b - Ax_s = r_0 - AW_s d = L_{s+1}((r_0)_{p_1} e_1^{(s+1)} - \bar{H}_s d).$$

Since L_{s+1} is not orthogonal, as CMRH, by defining $\bar{d}$ as

$$\bar{d} = \underset{d \in \mathbb{R}^s}{\operatorname{argmin}} \parallel (r_0)_{p_1} e_1^{(s+1)} - \bar{H}_s d \parallel,$$

the approximate solution x_s can be written as

$$x_s = x_0 + W_s \bar{H}_s^{\dagger} (r_0)_{p_1} e_1^{(s+1)}.$$

In this method, as augmented CMRH algorithm, the needed approximate eigenvectors of A can be found by using the subspace spanned by the columns of W_s and solving the small generalized eigenvalue problem (10).

Putting these results together gives the Algorithm 3.

Algorithm 3. One restarting cycle i of the CMRH-E(m,k)

Let $\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_k$ *be given harmonic Ritz vectors.*
Compute $r_i = b - Ax_i$ *and* $s = m + k$. *Set* $p = [1, 2 \ldots, n]^T$.
Determine i_0 *such that* $|(r_i)_{i_0}| = \|r_i\|_\infty$, $\beta = (r_i)_{i_0}$, $l_1 = r_i/\beta$, $p_1 \leftrightarrow p_{i_0}$.
For $j = 1, \ldots, s$
    $u = \begin{cases} Al_j & \textit{if } j \leq m \\ A\tilde{y}_{j-m} & \textit{otherwise.} \end{cases}$
    For $t = 1, \ldots, j$
        $h_{t,j} = (u)_{p_t}$,
        $u = u - h_{t,j} l_t$,
    end
    If ($u \neq 0$) *then*
        Determine $i_0 \in \{j+1, \ldots, n\}$ *such that* $|(u)_{p_{i_0}}| = \|(u)_{p_{j+1}:p_n}\|_\infty$,
        $h_{j+1,j} = (u)_{p_{i_0}}$, $l_{j+1} = u/h_{j+1,j}$, $p_{j+1} \leftrightarrow p_{i_0}$
    else
        $h_{j+1,j} = 0$, *Stop.*
    end
end
Set $L_{s+1} = [l_1, l_2, \ldots, l_{s+1}]$, $W_s = [l_1, \ldots, l_m, \tilde{y}_1, \ldots, \tilde{y}_k]$, $\bar{H}_s = \{h_{i,j}\}_{1 \leq i \leq j+1; 1 \leq j \leq s}$
Compute $x_{i+1} = x_i + W_s \hat{d}$, *where* $\hat{d}$ *minimizes* $\parallel \beta e_1^{(s+1)} - \bar{H}_s d \parallel$, $d \in \mathbb{R}^s$,
Solve the generalized eigen problem $\bar{H}_s^T L_{s+1}^T L_{s+1} \bar{H}_s g_j = \tilde{\theta}_j \bar{H}_s^T L_{s+1}^T W_s g_j$ *for the appropriate* g_j *and form* $\tilde{y}_j = W_s g_j$, *for* $j = 1, 2, \ldots, k$.

4 CMRH with deflated restarting

The general idea of deflation is to split the approximation space into two complementary subspaces such that the linear system projected onto one of these subspaces, referred to as the deflated linear system, will be easier to solve iteratively than the original linear system (1). These subspaces can be chosen in different ways. The Krylov subspace method is then confined in one of this subspace, by projecting the initial residual into this space and by replacing A by its restriction to this space. If the projection operator is chosen properly, the deflated linear system will be easier to solve iteratively than the original linear system. We combine simultaneously deflation and augmentation in the CMRH method. In this case, the search space $\mathcal{K}$ will be

$$\mathcal{K} = \mathcal{K}_m(\hat{A}, \hat{r}_0) + \mathcal{U}_k,$$

where $\mathcal{U}_k$ is the augmentation space of dimension k, $\mathcal{K}_m(\hat{A}, \hat{r}_0)$ represents the deflated Krylov subspace, $\hat{A}$ refers to the deflated operator, and $\hat{r}_0$ refers to the deflated residual. Given any initial guess x_0 and $s = m + k$, we consider an approximation solution of the form

$$x_s \in x_0 + \mathcal{K}_m(\hat{A}, \hat{r}_0) + \mathcal{U}_k.$$

This implies the following relation for the residual

$$r_s \in r_0 + A\mathcal{K}_m(\hat{A}, \hat{r}_0) + A\mathcal{U}_k.$$

As in [31]; we select $\mathcal{U}_k$ as an approximate invariant subspace and update this subspace at the end of each cycle. Let U_k be an $n \times k$ matrix whose columns vectors form a basis of the approximate invariant subspace $\mathcal{U}_k$. Assume that $Z = AU_k$, then the matrix $E := Z^T Z$ is nonsingular. We define the $n \times n$ matrices

$$Q := ZE^{-1}Z^T, \qquad P := I_n - Q. \tag{11}$$

We note that $P^2 = P$, $PAU_k = 0$, and $(AU_k)^T P = 0$, so, P is the projection on $(A\mathcal{U}_k)^\perp$ along $A\mathcal{U}_k$.

Using matrices (11) and matrix U_k, we set up the deflated system

$$\hat{A}x = \hat{b}, \tag{12}$$

where $\hat{A} := PA$ and $\hat{b} := Pb$. We point out that $\hat{A}$ is completely determined by A and the choice of the matrix U_k. Also, the system (12) is consistent, since it results from a left-multiplication of the consistent matrix equation $Ax = b$ with P.

Since $PAU_k = 0$, PA is singular, hence it is important to analyze the possibilities of a break down when solving the linear system (12). In the next subsection, we show that when CMRH is used to solve the deflated system (12), as GMRES, a break down can not occur if the condition $\mathcal{N}(PA) \cap \mathcal{R}(PA) = \{0\}$ holds.

By using $\hat{r}_0 = \hat{b} - \hat{A}x_0$ and the Hessenberg process (with pivoting) started with $l_1 = \hat{r}_0/(\hat{r}_0)_{p_1}$, where $|(\hat{r}_0)_{p_1}| = \| \hat{r}_0 \|_\infty$, we can construct the basis $L_m = [l_1, l_2, \ldots, l_m]$ for the Krylov subspace $\mathcal{K}_m(\hat{A}, \hat{r}_0) = \mathrm{span}\{\hat{r}_0, \hat{A}\hat{r}_0, \ldots, \hat{A}^{m-1}\hat{r}_0\}$. We have also the Hessenberg relation

$$\hat{A}L_m = L_{m+1}\bar{H}_m, \tag{13}$$

where $\bar{H}_m$ is an $(m+1)\times m$ upper Hessenberg matrix. Hence the approximate solution x_s from the affine space $x_0+\mathcal{K}_m(\hat{A},\hat{r}_0)+\mathcal{U}_k$ can be written as

$$x_s = x_0 + L_m k_s + U_k c_s,$$

with coordinate vectors $k_s \in \mathbb{R}^m$ and $c_s \in \mathbb{R}^k$. So, we have

$$r_s = b - Ax_s = r_0 - AL_m k_s - AU_k c_s.$$

Let $\beta = (\hat{r}_0)_{p_1}$. From (13), $Z = AU_k$, and $\hat{r}_0 = Pr_0 = (I_n - Q)r_0$, we have

$$\begin{aligned} r_s &= \beta l_1 + Qr_0 - (\hat{A}+QA)L_m k_s - Zc_s \\ &= \beta l_1 + ZE^{-1}Z^T r_0 - L_{m+1}\bar{H}_m k_s - ZE^{-1}Z^T AL_m k_s - Zc_s \\ &= [Z \quad L_{m+1}]B_s, \end{aligned}$$

where

$$B_s = \begin{bmatrix} E^{-1}Z^T r_0 \\ e_1^{(m+1)}\beta \end{bmatrix} - \begin{bmatrix} I_k & E^{-1}C_m \\ 0 & \bar{H}_m \end{bmatrix} \begin{bmatrix} c_s \\ k_s \end{bmatrix},$$

with $C_m = Z^T AL_m \in \mathbb{R}^{k\times m}$. Since $[Z \quad L_{m+1}]$ has not orthonormal columns, for computing c_s and k_s, we impose the following minimizing condition on the residual vectors r_s

$$\min \parallel B_s \parallel = \min_{k_s\in\mathbb{R}^m, c_s\in\mathbb{R}^k} \parallel \begin{bmatrix} E^{-1}Z^T r_0 \\ e_1^{(m+1)}\beta \end{bmatrix} - \begin{bmatrix} I_k & E^{-1}C_m \\ 0 & \bar{H}_m \end{bmatrix} \begin{bmatrix} c_s \\ k_s \end{bmatrix} \parallel . \tag{14}$$

This problem decouples into an $(m+1)\times m$ least squares problem for k_s and an explicit formula for c_s:

$$\min_{k_s\in\mathbb{R}^m} \parallel \beta e_1^{(m+1)} - \bar{H}_m k_s \parallel, \qquad c_s := E^{-1}Z^T r_0 - E^{-1}C_m k_s.$$

We observe that the explicit inclusion of U_k can be omitted when instead we first construct the iterate $\hat{x}_m = x_0 + L_m k_s \in x_0 + \mathcal{K}_m(\hat{A},\hat{r}_0)$ by using the quasi minimal residual norm and then apply the correction $x_s = \hat{x}_m + U_k c_s$. We can easily show that the projected residuals are equal to the original ones.

To define the subspace $\mathcal{U}_k$ for the next cycle, first we use the subspace spanned by the columns of $W_s = [U_k \quad L_m]$ which satisfies the relation

$$AW_s = \hat{W}_{s+1}\bar{G}_s, \tag{15}$$

where

$$\hat{W}_{s+1} = [Z \quad L_{m+1}], \qquad \bar{G}_s = \begin{bmatrix} I_k & E^{-1}C_m \\ 0 & \bar{H}_m \end{bmatrix}. \tag{16}$$

By using (5) and (15), we compute the required harmonic Ritz pairs $(\tilde{\theta}_j, \tilde{y}_j)$, $j = 1, \ldots, s$, by solving the small generalized eigenvalue problem

$$\bar{G}_s^T \hat{W}_{s+1}^T \hat{W}_{s+1} \bar{G}_s g_j = \tilde{\theta}_j \bar{G}_s^T \hat{W}_{s+1}^T W_s g_j, \qquad \tilde{y}_j = W_s g_j. \tag{17}$$

Next, we store the k eigenvectors g_j associated with the smallest eigenvalues (in magnitude) $\tilde{\theta}_j$ in G_k and define $\tilde{Y}_k = W_s G_k$. By performing the LU factorization (with pivoting) of $\bar{G}_s G_k$, as $\bar{G}_s G_k = \hat{L}_k \hat{U}_k$, (with the permutation matrix $\hat{P}_k = [e_{p_1}^{(s+1)}, e_{p_2}^{(s+1)}, \ldots, e_{p_{s+1}}^{(s+1)}]^T$), we define

$$U_k^{new} = \tilde{Y}_k \hat{U}_k^{-1} \qquad \text{and} \qquad Z^{new} = \hat{W}_{s+1} \hat{L}_k.$$

These relations and (15) together imply that $AU_k^{new} = Z^{new}$.

Putting these results together gives the following algorithm.

Algorithm 4. One restart cycle i of the CMRH-DR

Let U_k and $Z = AU_k$ be given matrices.
Compute $r_i = b - Ax_i$ and $s = m + k$. Set $p = [1, 2, \ldots, n]^T$.
Compute $E = Z^T Z$, $Q = ZE^{-1}Z^T$, $P = I_n - Q$.
Compute $\hat{r}_i = Pr_i$ and $\hat{A} = PA$.
Determine i_0 such that $|(\hat{r}_i)_{i_0}| = \|\hat{r}_i\|_\infty$, $\beta = (\hat{r}_i)_{i_0}$, $p_1 \leftrightarrow p_{i_0}$, $c = \beta e_1$.
Perform m Hessenberg steps with $\hat{A}$, letting $l_1 = \hat{r}_0/\beta$ and generating L_{m+1}, $\bar{H}_m$, and $C_m = Z^T A L_m$.
Set $W_s = [U_k \quad L_m]$, $\hat{W}_{s+1} = [Z \quad L_{m+1}]$ and $\bar{G}_s = \begin{bmatrix} I_k & E^{-1}C_m \\ 0 & \bar{H}_m \end{bmatrix}$.
Solve $\min \| c - \bar{H}_m k_s \|$ for k_s.
Compute $c_s = E^{-1}Z^T r_0 - E^{-1}C_m k_s$.
Compute $x_{i+1} = x_i + L_m k_s + U_k c_s$, $r_{i+1} = b - Ax_{i+1}$.
Compute the k eigenvectors g_j associated with the smallest eigenvalues (in magnitude) $\tilde{\theta}_j$ of $\bar{G}_s^T \hat{W}_{s+1}^T \hat{W}_{s+1} \bar{G}_s g_j = \tilde{\theta}_j \bar{G}_s^T \hat{W}_{s+1}^T W_s g_j$ and store in G_k.
Compute $\tilde{Y}_k = W_s G_k$
Perform the LU factorization of $\bar{G}_s G_k$ as $\bar{G}_s G_k = \hat{L}_k \hat{U}_k$ and $\hat{P}_k = [e_{p_1}^{(s+1)}, e_{p_2}^{(s+1)}, \ldots, e_{p_{s+1}}^{(s+1)}]^T$
Compute $Z = \hat{W}_{s+1} \hat{L}_k$, $U_k = \tilde{Y}_k \hat{U}_k^{-1}$. (Then we have $Z = AU_k$)

For the first run, standard CMRH(s) is used and $W_s = L_s$, $\hat{W}_{s+1} = L_{s+1}$, and $\bar{G}_s = \bar{H}_s$ are produced with the Hessenberg process by the initial vector r_0.

4.1 CMRH for a singular systems

A deflated matrix $\hat{A}$ is singular if $U_k \neq 0$, and we have to discuss whether the application of CMRH to the deflated system yields a well defined sequence of iterates that terminates with a solution. The application of GMRES to such systems has been analyzed in [7, 17, 22]. As in [7]; we state the following lemma for the properties of CMRH applied to singular consistent systems.

Lemma 1. *Apply CMRH to (1) and suppose that $\dim \mathcal{K}_k = k$ for some $k \geq 0$. Then exactly one of the following holds:*
(i) $\dim A(\mathcal{K}_k) = k - 1$ and $A(x_0 + z) \neq b$ for every $z \in \mathcal{K}_k$;
(ii) $\dim A(\mathcal{K}_k) = k$, $\dim \mathcal{K}_{k+1} = k$, x_k is uniquely defined, and $Ax_k = b$;
(iii) $\dim A(\mathcal{K}_k) = k$, $\dim \mathcal{K}_{k+1} = k + 1$, x_k is uniquely defined, and $Ax_k \neq b$.

Proof. As shown in Lemma 2.1 in [7], we have $k-1 \leqslant \dim A(\mathcal{K}_k) \leqslant k$ for all $k \geq 0$. We have also $r_0 \notin A(\mathcal{K}_{k-1})$ if $k > 0$. If $\dim A(\mathcal{K}_k) = k-1$, then conclusions (ii) and (iii) can not hold. In this case, as in [7]; we can show that for every $z \in \mathcal{K}_k$, we have $A(x_0 + z) \neq b$, and (only) conclusion (i) holds.

If $\dim A(\mathcal{K}_k) = k$, from $A(\mathcal{K}_k) \subseteq \mathcal{K}_{k+1}$, we have $k = \dim A(\mathcal{K}_k) \leq \dim \mathcal{K}_{k+1} \leq k+1$. If $\dim \mathcal{K}_{k+1} = k$, then we must have $A(\mathcal{K}_k) = \mathcal{K}_{k+1}$ and, hence $r_0 \in A(\mathcal{K}_k)$ and $Al_k \in \mathcal{K}_k$, then $l_{k+1} = 0$. In this case, from (3), we have $AL_k = L_k H_k$, $\text{rank}(H_k) = k$, and consequently

$$(\bar{H}_k)^{\dagger} = ((H_k)^{-1}, 0). \tag{18}$$

So, the iterate x_k, defined by (4), can be written as follows

$$x_k = x_0 + L_k (H_k)^{-1} (r_0)_{p_1} e_1^{(k)}.$$

Using $AL_k = L_k H_k$ and the last equality, we have

$$\begin{aligned} r_k = b - Ax_k &= r_0 - (r_0)_{p_1} A L_k (H_k)^{-1} e_1^{(k)} \\ &= r_0 - (r_0)_{p_1} L_k H_k (H_k)^{-1} e_1^{(k)} = r_0 - (r_0)_{p_1} l_1 = 0. \end{aligned}$$

Thus $Ax_k = b$, and (only) conclusion (ii) holds. If $\dim \mathcal{K}_{k+1} = k+1$, then $l_{k+1} \neq 0$ in $AL_k = L_{k+1} H_k + h_{k+1,k} l_{k+1} (e_k^{(k)})^T$. It follows that the decomposition $AL_k = L_{k+1} \bar{H}_k$ exists, the columns of the matrix L_{k+1} form a basis of $\mathcal{K}_{k+1}$, and the matrix $\bar{H}_k$ is of full rank and the iterate x_k can be uniquely defined by (4). In this case, we have $r_0 \notin A(\mathcal{K}_k)$, $r_k \neq 0$, $Ax_k \neq b$ and (only) conclusion (iii) holds. □

Using this lemma, the next two theorems give condition under which the CMRH iterates converge safely to a solution of the system. The proof is similar to the ones of Theorem 2.2 in [7] and Theorem 4.1 in [16], so we omit them here.

Theorem 1. *If the CMRH method is applied to* (1)*, then, at some step, either*
(a) CMRH breaks down through rank deficiency of the least-squares problem

$$\min_{d \in \mathbb{R}^k} \| \bar{H}_k d - (r_0)_{p_1} e_1^{(k+1)} \|,$$

without determining a solution $x_k = x_0 + L_k d_k$ or
(b) CMRH determines a solution without breakdown and then breaks down at the next step through degeneracy of the Krylov subspace.

Theorem 2. *Consider an arbitrary matrix $\hat{A} \in \mathbb{C}^{n \times n}$ and a vector $\hat{b} \in \mathcal{R}(\hat{A})$ (i.e., the linear system $\hat{A}x = \hat{b}$ is consistent). Then the following conditions are equivalent:*
1. For each initial guess $x_0 \in \mathbb{R}^n$, the CMRH method applied to the linear equation $\hat{A}x = \hat{b}$ is well defined at each iteration step k and it terminates with a solution of the system.
2. $\mathcal{N}(\hat{A}) \cap \mathcal{R}(\hat{A}) = \{0\}$.

Finally, by using the above results, we can show that, just as for deflated GMRES [16], for each initial guess $x_0 \in \mathbb{R}^n$, the CMRH method applied to the singular consistent equation (12) is well defined at each iteration step and it terminates with a solution of the system when $\mathcal{U}_k$ is an invariant subspace, i.e., when $A\mathcal{U}_k = \mathcal{U}_k$.

5 Numerical expriments

In this section, we present some results of solving linear systems of the form $Ax = b$ to illustrate the performance of the proposed algorithms. The codes are written in the programming package MATLAB and tested on a Workstation Intel Corei3, 2.40GHz. For all problems, the initial vector is the zero vector. For all matrices, the right-hand side was taken to be a vector with entries having random values between 0 and 1. The Jacobi (or diagonal) preconditioner has been used for all the test problems. The stopping criterion $\|r_i\| < 10^{-8}\|r_0\|$ was used. The maximum allowed number of cycles is $kmax = 3000$. We compare CMRH($m + k$) with augmented-CMRH(m,k), CMRH-E(m,k), and CMRH-DR(m,k) methods.

For the first set of examples, we used the matrices

$$A_1(i,j) = \begin{cases} \epsilon, & \text{if} \quad i = j, \\ \frac{2\min(i,j)-1}{n-i+j}, & \text{if} \quad i \neq j, \end{cases}$$

with $n = 100$, $\epsilon = 0.1$, and $\epsilon = 0.0001$, and

$$A_2 = \begin{pmatrix} \epsilon & 1 & & & & \\ -1 & \epsilon & 1 & & & \\ & & \epsilon & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & \epsilon & 1 \\ & & & & -1 & \epsilon \end{pmatrix},$$

with $n = 100$, $\epsilon = 0.01$, and $\epsilon = 0.0001$ [6].

For the second set of experiments, we used some matrices from Matrix Market collection* for the matrix A. These matrices with their generic properties are given in Table 1. In Table 2, we give the number of cycles (Cycle), and the matrix-vector products (Mvp) required for convergence. The notation "×" means that the relative residual norms have not reached the accuracy 10^{-8} after 3000 cycles. The results presented in Table 2 indicate that the augmented-CMRH(m,k), CMRH-E(m,k), and CMRH-DR(m,k) are effective for these problems and they are much better than standard CMRH($m + k$). As we observe, these examples get better results with CMRH-DR(m,k) in terms of matrix-vector products (except for Sherman4 which has better results with augmented-CMRH(18,2)). In addition, using four approximate eigenvectors

Table 1: Test problem information.

Matrix\property	order	sym.	nnz
nos3	960	Yes	8402
cdde1	961	No	4681
Sherman1	1000	Yes	2375
Sherman4	1104	No	3786
Sherman5	3312	No	20793
Saylr4	3564	No	22316
poisson3Da	13514	No	352762

*National institute of Standards and Technology: Matrix Market. http://math.nist.gov/Matrix-Market.

Table 2: Cycles and matrix-vector products required for convergence.

			CMRH($m+k$)		augmented-CMRH(m,k)		CMRH-E(m,k)		CMRH-DR(m,k)	
Matrix	m	k	Cycle	Mvp	Cycle	Mvp	Cycle	Mvp	Cycle	Mvp
A_1 with	20	0	688	13760						
ϵ =0.1	18	2			125	2500	96	1920	99	1784
	16	4			51	1020	60	1200	47	756
A_1 with	20	0	63	1260						
ϵ=0.0001	18	2			17	340	26	520	16	290
	16	4			12	240	18	360	12	196
A_2 with	20	0	426	8520						
ϵ =0.01	18	2			70	1400	76	1520	65	1172
	16	4			42	840	46	920	35	564
A_2 with	20	0	577	11540						
ϵ =0.0001	18	2			77	1540	71	1420	60	1082
	16	4			41	820	49	980	36	580
Sherman1	20	0	69	1380						
	18	2			32	640	38	760	31	560
	16	4			22	440	24	480	21	340
Sherman4	20	0	19	380						
	18	2			7	140	8	160	8	146
	16	4			7	140	8	160	7	116
Sherman5	20	0	38	760						
	18	2			11	220	12	240	11	200
	16	4			11	220	12	240	11	180
cdde1	20	0	425	8500						
	18	2			13	260	22	440	12	218
	16	4			11	220	17	340	10	164
nos3	20	0	1118	22360						
	18	2			58	1160	59	1180	45	812
	16	4			23	460	41	820	19	308
poisson3Da	20	0	23	460						
	18	2			13	260	13	260	13	236
	16	4			13	260	13	260	12	196
Saylr4	20	0	×	×						
	18	2			×	×	2233	44660	1471	26480
	16	4			2710	54200	×	×	768	12292

($m=16$ and $k=4$) gives the lowest number of cycles and matrix-vector products for all test matrices (except for matrix Saylr4 which have better results with CMRH-E(18,2)).

For the matrices Sherman1, Sherman4, Sherman5, and Saylr4, the relative residual norms ($\|r_i\|/\|r_0\|$) are plotted against the number of matrix-vector products. See figures 1 and 2 for the graph of convergence of the methods. These figures show that augmented-CMRH(17,3), CMRH-E(17,3), and CMRH-DR(17,3) compete well for these examples and are much better than CMRH(20). CMRH-DR is also better than augmented-CMRH and CMRH-E in terms of matrix-vector products. The augmented-CMRH(17,3) and CMRH-E(17,3) have similar convergence. Finally, we mention that, for Saylr4 (Fig. 2 (right)), CMRH(20) is not convergence in 3000 cycles and reaches the relative residual norm of 0.0023, while augmented-CMRH(17,3), CMRH-E(17,3), and CMRH-DR(17,3) need 25820, 23240, and 14810 Mvps and have the relative residual norms of 9.8022e-09, 9.4538e-09, and 9.8836e-09, respectively.

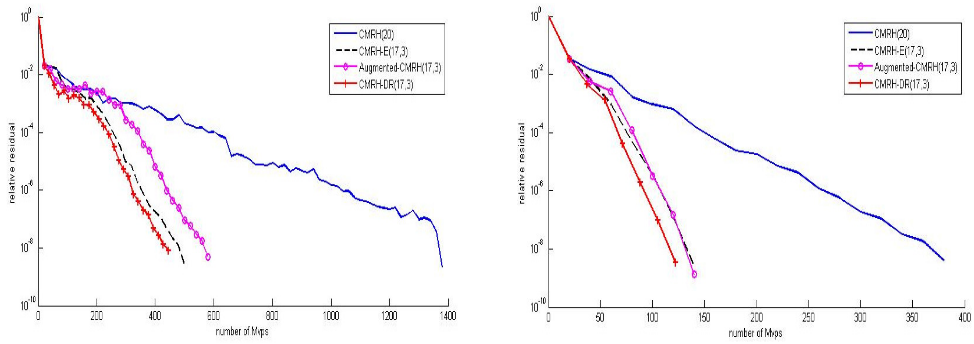

Figure 1: The relative residual norm against matrix-vector products for the matrices Sherman1 (left) and Sherman4 (right).

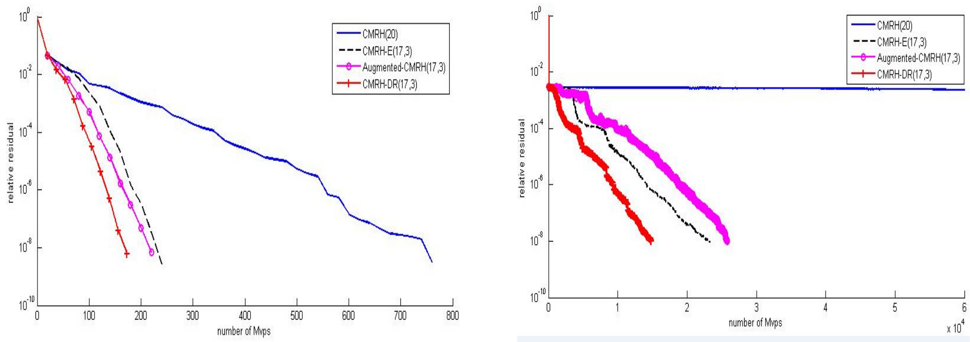

Figure 2: The relative residual norm against matrix-vector products for matrices Sherman5 (left) and Saylr4 (right).

6 Conclusions

In this paper, we have described three methods that accelerate the convergence of CMRH(m). The techniques are straightforward and easy to implement. Numerical experiments show that the new methods can shrink the slow convergence phase and thus considerably accelerate the convergence of CMRH. The methods are not really needed for easy problems where few restarts are used. The experiments show that the results of CMRH-DR algorithm are often better than those of augmented-CMRH and CMRH-E algorithms.

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