Applied Numerical Mathematics 99 (2016) 137–150

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Deflated and augmented global Krylov subspace methods for the matrix equations

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ARTICLE INFO

Article history:
Received 30 October 2014
Received in revised form 19 June 2015
Accepted 9 August 2015
Available online 11 September 2015

Keywords:
Matrix equation
Global methods
Deflated and augmented methods
Gl-CG
Gl-GMRES
Gl-MINRES

ABSTRACT

Global Krylov subspace methods are among the most efficient algorithms to solve matrix equation $AX = B$. Deflation and augmentation techniques are used to accelerate the convergence of Krylov subspace methods. There are two different approaches for deflated and augmented methods: an augmentation space is applied explicitly in every step, or the global method is used for solving a projected problem and then a correction step is applied at the end. In this paper, we present a framework of deflation and augmentation approaches for accelerating the convergence of the global methods for the solution of nonsingular linear matrix equations $AX = B$. Then, we define deflated and augmented global algorithms. Also, we analyze the deflated and augmented global minimal residual and global orthogonal residual methods. Finally, we present numerical examples to illustrate the effectiveness of different versions of the new algorithms.

1. Introduction

Many applications in science and engineering require the solution of a matrix equation

$$AX = B, \tag{1}$$

where A is an $m \times m$ real matrix and B and X are $m \times s$ rectangular matrices with $s \ll m$.

For solving matrix equation (1), some block Krylov subspace methods have been developed in the past years. O'Leary [22] presented the block conjugate gradient (Bl-CG) algorithm for symmetric positive definite problems. An adaptive block Lanczos algorithm and a block version of MINRES method were developed in [4] when the matrix is symmetric. In [26], the block generalized minimal residual (Bl-GMRES) algorithm was established.

Recently, global Krylov subspace methods have been generated by projecting globally the initial matrix residual onto a block Krylov subspace. Jbilou et al. [14] presented the global full orthogonalization method (Gl-FOM) and the global GMRES method (Gl-GMRES) for the nonsymmetric matrix equation (1). In the case where the coefficient matrix A is diagonalizable and nonsymmetric, Bellalij et al. [1] obtained some new convergence results for Gl-GMRES. Gu and Yang [12] presented the global semi-conjugate direction algorithms. For symmetric positive definite matrix A, the Gl-CG method [7] is presented.

In Bl-GMRES, the chosen block size for $\mathcal{V}_n$ (Arnoldi basis for the Krylov subspace $K_n(A, R_0)$) should be small, such as $n = 2$, since Bl-GMRES becomes, in each restart, time-consuming in computation when n is large. While for Gl-GMRES, it

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http://dx.doi.org/10.1016/j.apnum.2015.08.010
0168-9274/

is appropriate to take the block size for basis $\mathcal{V}_n$ larger, such as $n = 25$ [7]. Example 1 in [29] shows that for large n, the iteration steps are reduced but the required CPU-time increases. Also, Gl-GMRES for large n is more effective than Bl-GMRES. In the block methods, to delete linearly or almost linearly dependent vectors generated during the iterations, a deflation procedure is often used [9]. However, the global methods do not suffer from dependence of vectors during the iterations. Therefore, no deflation procedure is used to delete linearly or almost linearly dependent vectors. Examples in [15,25,29,31,32,34] show that the global methods are effective, as compared to block methods, for solving large and sparse matrix equations. In general, block methods are more effective for dense linear systems than for sparse linear systems [16].

Deflation and augmentation are two techniques for accelerating the convergence of Krylov subspace methods. In augmentation approaches, the search space of the method is made larger by an appropriately selected subspace [10]. Since eigenvalues of the operator close to zero incline to reduce the speed of convergence of the Krylov subspace methods [3], these eigenvalues are essentially deflated from the spectrum of the matrix, with adding the corresponding eigenvectors to the search space. In deflation, for removing components that decelerate convergence, the linear system $Ax = b$ is multiplied with a properly selected projection operator [10].

The first deflation and augmentation techniques for solving linear systems were presented by Nicolaides [21] and Dostál [5]. For symmetric positive definite matrix A, Saad et al. [24] described a deflated version of the CG algorithm. Also, Vuik et al. [27] applied deflated CG with incomplete Cholesky preconditioning for the solution of a class of layered problems with extreme contrasts in the coefficients. Nabben and Vuik [19,20] presented similarities between the domain decomposition methods and deflation approach. In 1990, Morgan [18] considered GMRES with an augmented basis but not with explicit deflation. In [13], a recent superior analysis of these methods together with detailed references and historical explanations can be found. Also, for linear systems with non-Hermitian matrices, applications of deflated Krylov subspace methods with orthogonal and oblique projections were presented in [8].

We can merge simultaneously deflation and augmentation in a single Krylov subspace method. In this case, the search space of the Krylov subspace method will be

$$S_n = \mathcal{U} + \widetilde{K}_n,$$

where $\mathcal{U}$ is the augmentation space and $\widetilde{K}_n$ represents the deflated Krylov subspace.

In this paper, we consider global minimal residual (Gl-MR) [6] methods including all global methods that are theoretically equivalent to Gl-GMRES and global orthogonal residual (Gl-OR) [2] methods containing the methods that are theoretically equivalent to Gl-FOM. Then, we present an extension of the framework of Gaul et al. [10] to the global methods for solving matrix equation (1) and define a deflated and augmented global algorithm.

This paper is organized as follow: In Section 2, we review some definitions and properties which are utilized throughout this article. In Section 3, we present a framework for deflated and augmented global Krylov subspace methods for the solution of matrix equation (1) and define a deflated and augmented global algorithm. Section 4 is devoted to employing deflation and augmentation for global OR-type methods. Also, a deflated and augmented version of the global MR-type methods and particularly Gl-MINRES is discussed in Section 5. In Section 6, numerical examples are presented. Finally, some concluding remarks are given in Section 7.

We use the following notations. For two matrices Y and Z in $\mathbb{R}^{m\times s}$, we define the inner product $< Y, Z >_F = tr(Y^T Z)$ where $tr(Y^T Z)$ denotes the trace of the matrix $Y^T Z$. The associated norm is the Frobenius norm denoted by $\|.\|_F$. A system of matrices of $\mathbb{R}^{m\times s}$ is said to be F-orthonormal if it is orthonormal with respect to $< ., . >_F$. We denote the null space and the range space of matrix A by $\mathcal{N}(A)$ and $\mathcal{R}(A)$, respectively.

2. Definitions and properties

In this section, we give definitions and properties of the Kronecker product and the $\diamond$ product. Also, we briefly review the global OR-type methods and the global MR-type methods.

2.1. The Kronecker product and the $\diamond$ product

The Kronecker product of matrices A and B is given by $A \otimes B = [a_{ij}B]$. For this product, we have the following properties [30]:

(1) $(A \otimes B)^T = A^T \otimes B^T$.
(2) $(A \otimes B)(C \otimes D) = (AC \otimes BD)$.
(3) $tr(A \otimes B) = tr(A)tr(B)$.

In the following we recall the product denoted by $\diamond$ [2]:

Definition 2.1. Let $A = [A_1, A_2, \ldots, A_p]$ and $B = [B_1, B_2, \ldots, B_l]$ be matrices of dimension $n \times ps$ and $n \times ls$, respectively, where A_i and B_j $(i = 1, \ldots, p; j = 1, \ldots, l)$ are $n \times s$ matrices. Then the $p \times l$ matrix $A^T \diamond B$ is defined by:

$$A^T \diamond B = \begin{pmatrix} < A_1, B_1 >_F & < A_1, B_2 >_F & \dots & < A_1, B_l >_F \\ < A_2, B_1 >_F & < A_2, B_2 >_F & \dots & < A_2, B_l >_F \\ \vdots & \vdots & \vdots & \vdots \\ < A_p, B_1 >_F & < A_p, B_2 >_F & \dots & < A_p, B_l >_F \end{pmatrix}.$$

It is not difficult to prove the following remark.

Remark 2.2. For the $\diamond$ product, we have:

(1) If $s = 1$ then $A^T \diamond B = A^T B$.
(2) If $s = 1$, $p = 1$ and $l = 1$, then setting $A = u \in \mathbb{R}^n$ and $B = v \in \mathbb{R}^n$, we have $A^T \diamond B = u^T v \in \mathbb{R}$.
(3) The matrix $A = [A_1, A_2, \dots, A_p]$ is F-orthonormal if and only if $A^T \diamond A = I_p$.
(4) If $X \in \mathbb{R}^{n \times s}$, then $X^T \diamond X = \|X\|_F^2$.

We have the following properties for the $\diamond$ product.

Proposition 2.3. *(See [2].) Let $A, B, C \in \mathbb{R}^{n \times ps}$, $D \in \mathbb{R}^{n \times n}$, $L \in \mathbb{R}^{p \times p}$ and $\alpha \in \mathbb{R}$. Then*

(1) $(A + B)^T \diamond C = A^T \diamond C + B^T \diamond C$.
(2) $A^T \diamond (B + C) = A^T \diamond B + A^T \diamond C$.
(3) $(\alpha A)^T \diamond C = \alpha (A^T \diamond C)$.
(4) $(A^T \diamond B)^T = B^T \diamond A$.
(5) $(DA)^T \diamond B = A^T \diamond (D^T B)$.
(6) $A^T \diamond (B(L \otimes I_s)) = (A^T \diamond B)L$.

2.2. The global OR-type methods

We consider the block Krylov subspace of $\mathbb{R}^{m \times s}$ [7] spanned by the matrices $V, AV, \dots, A^{n-1}V$ of the form

$$K_n(A, V) = span\{V, AV, \dots, A^{n-1}V\},$$

where A is an $m \times m$ matrix and V is an $m \times s$ matrix. Note that $Z \in K_n(A, V)$ means that

$$Z = \sum_{i=1}^{n} y_i A^{i-1} V = [V, AV, \dots, A^{n-1}V](y \otimes I_s),$$

where $y = [y_1, y_2, \dots, y_n] \in \mathbb{R}^n$.

Now, we consider matrix equation (1) with initial residual $R_0 = B - AX_0$ where X_0 is an initial $m \times s$ matrix. At step n, a global OR-type method [2] generates approximation X_n^{OR} such that

$$X_n^{OR} - X_0 = Z_n \in K_n(A, R_0), \tag{2}$$

and residual R_n^{OR} satisfies the orthogonality relation

$$R_n^{OR} = R_0 - AZ_n \perp_F K_n(A, R_0), \tag{3}$$

where the notation $\perp_F$ means orthogonality with respect to the inner product $< ., . >_F$. Note that R_n^{OR} is obtained by projecting R_0 onto $AK_n(A, R_0)$ along to the F-orthogonal of the Krylov subspace $K_n(A, R_0)$.

We consider the F-orthonormal basis V_n, constructed with the global Arnoldi algorithm [14]. From relation (2), we conclude that

$$X_n^{OR} = X_0 + V_n(y_n \otimes I_s), \tag{4}$$

where vector y_n is obtained by imposing orthogonality condition (3). By substituting (4) in R_n^{OR}, we obtain

$$R_n^{OR} = R_0 - AV_n(y_n \otimes I_s).$$

2.3. The global MR-type methods

A global-MR type method [6] constructs, at step n, the approximation X_n^{MR} satisfying the following two relations

$$X_n^{MR} - X_0 \in K_n(A, R_0), \tag{5}$$

and

$$R_n^{MR} \perp_F K_n(A, AR_0). \tag{6}$$

From (5), we obtain

$$X_n^{MR} = X_0 + V_n(y_n \otimes I_s), \tag{7}$$

where vector y_n is obtained by imposing orthogonality condition (6). The F-orthonormal basis V_n for Krylov subspace $K_n(A, AR_0)$ is constructed with the global Arnoldi algorithm. Note that R_n^{MR} is obtained by projecting R_0 onto $AK_n(A, R_0)$ along to the F-orthogonal of the Krylov subspace $K_n(A, AR_0)$. By substituting (7) in R_n^{MR}, we get

$$R_n^{MR} = R_0 - AV_n(y_n \otimes I_s).$$

Since, the global MR-type method is an orthogonal projection method onto the Krylov subspace $K_n(A, AR_0)$, we have the minimization property

$$\|R_n^{MR}\|_F = \min_{Z \in K_n(A,R_0)} \|R_0 - AZ\|_F.$$

3. A framework for deflated and augmented global Krylov subspace methods

In this section, we present a general framework for deflated and augmented global Krylov subspace methods for the solution of matrix equation (1). Given an initial guess $X_0 \in \mathbb{R}^{m\times s}$, an n-dimensional subspace S_n of $\mathbb{R}^{m\times s}$, we consider an approximation X_n to the solution X of the form

$$X_n \in X_0 + S_n, \tag{8}$$

so that the corresponding residual satisfies

$$R_n := B - AX_n \perp_F \mathcal{B}S_n, \tag{9}$$

where $\mathcal{B} \in \mathbb{R}^{m\times m}$ is a nonsingular matrix. When A is symmetric positive definite, $\mathcal{B} = I$ and the search space S_n is the nth block Krylov subspace generated by A and the initial residual $R_0 := B - AX_0$, then (8) and (9) mathematically characterize the Gl-CG method. If $\mathcal{B} = A$ and A is nonsingular, then (8) and (9) mathematically characterize the Gl-GMRES method.

Now, we suppose that the search space S_n is augmented with a space $\mathcal{U}$:

$$S_n = \widetilde{K}_n + \mathcal{U}. \tag{10}$$

Here, $\mathcal{U}$ is called the augmentation space and the subspace $\widetilde{K}_n$ has dimension n. Let matrix $U \in \mathbb{R}^{m\times k}$ be such that

$$E_{\mathcal{B}} := U^T\mathcal{B}^T AU \in \mathbb{R}^{k\times k} \tag{11}$$

is nonsingular. We define the $m \times m$-matrices

$$\begin{cases} Q_{\mathcal{B}} := UE_{\mathcal{B}}^{-1}U^T, \\ P_{\mathcal{B}} := I - AQ_{\mathcal{B}}\mathcal{B}^T, \\ \widetilde{P}_{\mathcal{B}} := I - Q_{\mathcal{B}}\mathcal{B}^T A. \end{cases} \tag{12}$$

The following lemma states some basic properties of the matrices $P_{\mathcal{B}}$ and $\widetilde{P}_{\mathcal{B}}$. The proof of these properties is straightforward, and is therefore omitted.

Lemma 3.1. *We consider a k-dimensional space $\mathfrak{U}$ and denote by U a matrix whose columns form a basis of $\mathfrak{U}$. Also, we suppose that matrix $E_{\mathcal{B}} := U^T\mathcal{B}^T AU$ is nonsingular. Then the matrices (12) are well defined and the following statements hold:*

(1) $P_{\mathcal{B}}^2 = P_{\mathcal{B}}$, $P_{\mathcal{B}}AU = 0$, *and* $U^T\mathcal{B}^T P_{\mathcal{B}} = 0$, *i.e., $P_{\mathcal{B}}$ is the projection onto $(\mathcal{B}\mathfrak{U})^{\perp}$ along $A\mathfrak{U}$.*
(2) $\widetilde{P}_{\mathcal{B}}^2 = \widetilde{P}_{\mathcal{B}}$, $\widetilde{P}_{\mathcal{B}}U = 0$, *and* $U^T\mathcal{B}^T A\widetilde{P}_{\mathcal{B}} = 0$, *i.e., $\widetilde{P}_{\mathcal{B}}$ is the projection onto $(A^T\mathcal{B}\mathfrak{U})^{\perp}$ along $\mathfrak{U}$.*
(3) $P_{\mathcal{B}}A = A\widetilde{P}_{\mathcal{B}}$.

The following theorem shows that solving a deflated matrix equation, we can obtain a solution X_n of matrix equation (1) such that conditions (8) and (9) are satisfied.

Theorem 3.2. *Let the assumptions of Lemma 3.1 be satisfied and subspace $\widetilde{K}_n$ of $\mathbb{R}^{m\times s}$ has dimension n. We denote by $V_n = [V_n^{(1)}, V_n^{(2)}, \ldots, V_n^{(n)}]$ a matrix whose blocks $V_n^{(i)} \in \mathbb{R}^{m\times s}$ form a basis of $\widetilde{K}_n$. Furthermore, we consider $\mho = \{U_i e_j^T \in \mathbb{R}^{m\times s}, i = 1,\ldots,k, j = 1,\ldots,s\}$ where U_i is ith column of matrix U and e_j is the jth canonical basis vector in $\mathbb{R}^s$. Also, we suppose a ks-dimensional space $\mathcal{U}$ of $\mathbb{R}^{m\times s}$ such that $\mho$ is a basis of it. Let $B,\ X_0 \in \mathbb{R}^{m\times s}$ be arbitrary matrices.*

Now, we consider the solution $\widehat{X}_n$ of the matrix equation $\widehat{A}X = \widehat{B}$ where $\widehat{A} := P_{\mathcal{B}}A$ and $\widehat{B} := P_{\mathcal{B}}B$, such that

$$\widehat{X}_n \in X_0 + \widetilde{K}_n, \tag{13}$$

$$\widehat{R}_n := \widehat{B} - \widehat{A}\widehat{X}_n \perp_F \mathcal{B}\widetilde{K}_n, \tag{14}$$

for $n \geq 1$ in the sense that

$$X_n = \widetilde{P}_{\mathcal{B}}\widehat{X}_n + Q_{\mathcal{B}}\mathcal{B}^T B, \tag{15}$$

$$R_n = \widehat{R}_n. \tag{16}$$

Then

$$X_n \in X_0 + \widetilde{K}_n + \mathcal{U}, \tag{17}$$

$$R_n = B - AX_n \perp_F \mathcal{B}\widetilde{K}_n + \mathcal{B}\mathcal{U}. \tag{18}$$

Proof. From (15) and (16) and by using matrices (12), we have

$$\begin{aligned} R_n &= \widehat{B} - \widehat{A}\widehat{X}_n = P_{\mathcal{B}}(B - A\widehat{X}_n) \\ &= B - A\widehat{X}_n - AQ_{\mathcal{B}}\mathcal{B}^T B + AQ_{\mathcal{B}}\mathcal{B}^T A\widehat{X}_n \\ &= B - A(\widetilde{P}_{\mathcal{B}}\widehat{X}_n + Q_{\mathcal{B}}\mathcal{B}^T B) \\ &= B - AX_n. \end{aligned}$$

Therefore, the first orthogonality condition in (18) is satisfied by using (16) and condition (14). Also, we note that relations (13) and (14) mean that

$$\widehat{X}_n = X_0 + V_n(y_n \otimes I_s),$$

$$\widehat{R}_n = P_{\mathcal{B}}(B - A\widehat{X}_n),$$

for some vector $y_n \in \mathbb{R}^n$. Substituting $\widehat{X}_n$ and $\widehat{R}_n$ in (15) and (16) and using matrices (12), get

$$\begin{aligned} X_n &= (I - UE_{\mathcal{B}}^{-1}U^T\mathcal{B}^T A)(X_0 + V_n(y_n \otimes I_s)) + UE_{\mathcal{B}}^{-1}U^T\mathcal{B}^T B \\ &= X_0 + V_n(y_n \otimes I_s) + U(E_{\mathcal{B}}^{-1}U^T\mathcal{B}^T(R_0 - AV_n(y_n \otimes I_s))), \\ R_n &= (I - AUE_{\mathcal{B}}^{-1}U^T\mathcal{B}^T)(R_0 - AV_n(y_n \otimes I_s)) \\ &= R_0 - AV_n(y_n \otimes I_s) - AU(E_{\mathcal{B}}^{-1}U^T\mathcal{B}^T(R_0 - AV_n(y_n \otimes I_s))). \end{aligned}$$

Then, assuming

$$U_n := E_{\mathcal{B}}^{-1}U^T\mathcal{B}^T(R_0 - AV_n(y_n \otimes I_s))$$

gives

$$X_n = X_0 + V_n(y_n \otimes I_s) + UU_n, \tag{19}$$

$$R_n = R_0 - AV_n(y_n \otimes I_s) - AUU_n. \tag{20}$$

From (19), we have

$$X_n \in X_0 + \widetilde{K}_n + \mathcal{U}.$$

Also for (20), the following relation is satisfied

$$(\mathcal{B}U)^T R_n = 0,$$

so, for $i = 1,\ldots,k$ and $j = 1,\ldots,s$

$$e_j U_i^T \mathcal{B}^T R_n = 0.$$

Then

$$R_n \perp_F \mathcal{B}\mathcal{U}.$$

Therefore, conditions (17) and (18) are satisfied. □

For $s = 1$ (single right-hand side), theoretically, the deflated and augmented global method is equivalent to the deflated and augmented method in [10].

Note that in the proof of Theorem 3.2, we use from the fact that for each A and B in $\mathbb{R}^{m\times s}$, we have

$$A^T B = 0 \Rightarrow < A, B >_F = 0,$$

while for $s = 1$, we give

$$A^T B = 0 \Leftrightarrow < A, B >_F = 0.$$

Also using Remark 2.2, F-orthogonality ($\perp_F$) in the case of $s = 1$ reduces to Euclidean orthogonality. Therefore, we have the following corollary.

Corollary 3.3. *Using the notations of Theorem 3.2 for $s = 1$, the following two sets of conditions*

$$X_n \in X_0 + \widetilde{K}_n + \mathcal{U},$$
$$R_n = B - AX_n \perp \mathcal{B}\widetilde{K}_n + \mathcal{B}\mathcal{U}$$

and

$$\widehat{X}_n \in X_0 + \widetilde{K}_n,$$
$$\widehat{R}_n := \widehat{B} - \widehat{A}\widehat{X}_n \perp \mathcal{B}\widetilde{K}_n,$$

are equivalent for $n \geq 1$ in the sense that

$$X_n = \widetilde{P}_{\mathcal{B}}\widehat{X}_n + Q_{\mathcal{B}}\mathcal{B}^T B,$$
$$R_n = \widehat{R}_n.$$

Proof. See [10]. □

Conditions (17) and (18), where the augmentation space $\mathcal{U}$ is explicitly contained in the search space, represent the explicit deflated and augmented method. In conditions (13) and (14), the explicit inclusion of $\mathcal{U}$ is replaced by a suitable projection of a restricted problem: we first construct iterations $\widehat{X}_n \in X_0 + \widetilde{K}_n$ without components in $\mathcal{U}$ such that the projected residuals $\widehat{R}_n = P_{\mathcal{B}}(B - A\widehat{X}_n)$ satisfy the simplified condition of (14). Then, we apply the final correction step (15). Interestingly, the projected residuals are equal to the original ones. We call this the implicit deflated and augmented method. According to its definition, $\widehat{R}_n$ is the residual of the approximate solution $\widehat{X}_n$ of the projected or deflated matrix equation

$$\widehat{A}\widehat{X}_n = \widehat{B}, \tag{21}$$

where $\widehat{A} = P_{\mathcal{B}}A$, $\widehat{B} = P_{\mathcal{B}}B$.

Thus, we can consider $\widetilde{K}_n := K_n(\widehat{A}, \widehat{R}_0)$ and solve matrix equation (21) with conditions (13) and (14) using the global Krylov subspace methods. Note that matrices $\widehat{A}$ and U are in general unrelated.

So far we have not specified the matrices $\widehat{A}$ and $\widehat{R}_0 := \widehat{B} - \widehat{A}\widehat{X}_0$. In the following sections we will discuss suitable choices for $\widehat{A}$ and $\widehat{R}_0$ depending the properties of the matrix A.

Using the implicit approach of Theorem 3.2, we can obtain a deflated and augmented global (Def-Aug-Global) algorithm.

Algorithm 1 *(Def-Aug-Global algorithm).*

1. function $[n, X_n, R_n] =$ Def-Aug-Global$(A, B, \widehat{X}_0, U, \mathcal{B})$.
   input: $A, B, \widehat{X}_0, U, \mathcal{B}$.
   code for $E_{\mathcal{B}}, Q_{\mathcal{B}}, P_{\mathcal{B}}, \widetilde{P}_{\mathcal{B}}$ [see (12)].
   output: approximate solution X_n of $AX = B$; corresponding n, R_n.
2. $\widehat{A} = P_{\mathcal{B}}A$, $\widehat{B} = P_{\mathcal{B}}B$.
3. $[n, \widehat{X}_n, \widehat{R}_n] =$ Global$(\widehat{A}, \widehat{B}, \widehat{X}_0)$ [apply global method to $\widehat{A}X = \widehat{B}$].
4. $X_n = \widetilde{P}_{\mathcal{B}}\widehat{X}_n + Q_{\mathcal{B}}\mathcal{B}^T B$, and $R_n = \widehat{R}_n$ [see (15) and (16)].

4. Deflated and augmented global OR-type method

In this section, we present deflated and augmented global OR-type methods. We choose $\mathcal{B} = I$ and some k-dimensional space $\mathfrak{U}$ with corresponding matrix U. If A is even symmetric positive definite, conditions (8) and (9) characterize deflated and augmented Gl-CG method. In this case, matrix $E_I = U^T AU$ is nonsingular, and the assumptions of Theorem 3.2 are satisfied. Hence, we present a framework for deflated and augmented Gl-CG method.

Using matrices (12) and matrix U, we set up the deflated matrix equation

$$\widehat{A}\widehat{X}_n = \widehat{B}, \tag{22}$$

where

$$\widehat{A} := P_I A, \quad \widehat{B} := P_I B,$$

here, $P_I = I - AU(U^T AU)^{-1}U^T$ as defined in (12) when $\mathcal{B} = I$. Moreover, $\widetilde{P}_I = P_I^T$. Clearly, the deflated matrix $\widehat{A}$ is singular, since P_I is a nontrivial projector if $0 < k < m$. Also, matrix equation (22) is consistent, since it results from a left-multiplication of the consistent matrix equation $AX = B$ with P_I. Note that $\widehat{A}$ is symmetric, and this matrix is also positive semidefinite, since

$$v^T \widehat{A} v = v P_I A v = v^T P_I (P_I A) v = v^T P_I (P_I A)^T v = v^T P_I A P_I^T v \geq 0$$

holds for any $v \in \mathbb{R}^m$.

We point out that $\widehat{A}$ as defined in (22) is completely determined by A and the choice of the matrix U. (Recall that in Theorem 3.2, the matrices $\widehat{A}$ and U can be unrelated.)

The nth step of the Gl-CG method applied to the deflated system (22) with the initial guess X_0 and the resulting initial residual $\widehat{R}_0 = \widehat{B} - \widehat{A}\widehat{X}_0$ is mathematically characterized by the following two conditions

$$\widehat{X}_n \in X_0 + K_n(\widehat{A}, \widehat{R}_0),$$
$$\widehat{R}_n = \widehat{B} - \widehat{A}\widehat{X}_n = P_I(B - A\widehat{X}_n) \perp_F K_n(\widehat{A}, \widehat{R}_0).$$

In the sense of relations (15) and (16), these conditions give conditions (17) and (18), namely

$$X_n \in X_0 + K_n(\widehat{A}, \widehat{R}_0) + \mathcal{U},$$
$$R_n = B - AX_n \perp_F K_n(\widehat{A}, \widehat{R}_0) + \mathcal{U},$$

where space $\mathcal{U}$ has dimension ks and set $\mathcal{O} = \{U_i e_j^T \in \mathbb{R}^{m\times s}, i = 1, \ldots, k, j = 1, \ldots, s\}$ forms a basis of it.

This is the starting point of the deflated and augmented Gl-CG method.

Now, we can define the effective condition number of the positive semidefinite matrix $P_I A$ denoted $\kappa_{eff}(P_I A)$, as the ratio of its largest to smallest strictly positive eigenvalues.

In deflated and augmented methods, we try to obtain a deflated matrix $P_I A$ whose effective condition number is smaller than the one of A, for example by eliminating the smallest eigenvalues of A.

We denote the t distinct eigenvalues of A ordered by increasing magnitude (i.e., values as they are real positive) by $\lambda_1 = \lambda_{\min}, \ldots, \lambda_t = \lambda_{\max}$. The union of eigenspaces associated with the smallest eigenvalues $\lambda_1, \ldots, \lambda_k$ of A is an invariant subspace and can be used for $\mathfrak{U}$. Since $P_I AU = 0_{m\times k}$, then $P_I A$ has k zero eigenvalues. We consider the orthogonal complement of U and denote it by $U^\perp$, i.e., $U^T Z = 0$ so that $P_I Z = Z$. Because A is symmetric positive definite, Z defines an invariant subspace associated with the eigenvalues $\lambda_{k+1}, \ldots, \lambda_t = \lambda_{\max}$. Then, we have $AZ = ZC$ for some nonsingular C. Consequently, we have $P_I AZ = P_I ZC = ZC$ so that Z is an invariant subspace of $P_I A$ associated with the same eigenvalues $\lambda_{k+1}, \ldots, \lambda_{\max}$. Therefore, we have

$$\kappa_{eff}(P_I A) = \frac{\lambda_{\max}}{\lambda_{k+1}}.$$

Thus, deflating with an invariant subspace cancels the corresponding eigenvalues, leaving the rest of the spectrum unchanged. If $\lambda_{k+1} \gg \lambda_{\min}$ the convergence of Gl-CG is significantly improved.

5. Deflated and augmented global MR-type method

In this section, we present deflated and augmented global MR-type methods. Assuming $\mathcal{B} = A$, the matrix $E_A = U^T A^T AU$ is nonsingular for any (nontrivial) space $\mathfrak{U}$. Thus, the assumptions of Theorem 3.2 are satisfied. We now consider the application of a global MR-type method to the deflated system

$$\widehat{A}X = \widehat{B}, \tag{23}$$

where $\widehat{A} := P_A A$ and $\widehat{B} := P_A B$.

Deflated matrix $\widehat{A} = P_A A$ is singular if $\mathfrak{U} \neq 0$ and matrix $P_A = AU(U^T A^T AU)^{-1} U^T A^T$ is symmetric. If we start the global MR-type method with an initial guess X_0 and the corresponding initial residual $\widehat{R}_0 = \widehat{B} - \widehat{A}X_0 = P_A(B - AX_0)$ then the iterations $\widehat{X}_n$ and the residuals $\widehat{R}_n$ are characterized by the two conditions

$$\widehat{X}_n \in X_0 + K_n(\widehat{A}, \widehat{R}_0),$$

and

$$\widehat{R}_n = \widehat{B} - \widehat{A}\widehat{X}_n \perp_F \widehat{A}K_n(\widehat{A}, \widehat{R}_0). \tag{24}$$

Let $V_n = [V_n^{(1)}, V_n^{(2)}, \ldots, V_n^{(n)}]$ be a matrix such that the matrices $V_n^{(i)}$, $i = 1, \ldots, n$ form a basis of $K_n(\widehat{A}, \widehat{R}_0)$. Condition (24) means that

$$\begin{aligned} 0 &= tr(V_n^{(i)T} \widehat{A}^T \widehat{R}_n) = tr(V_n^{(i)T} A^T P_A^T \widehat{R}_n) = tr(V_n^{(i)T} A^T P_A P_A (B - A\widehat{X}_n)) \\ &= tr(V_n^{(i)T} A^T P_A (B - A\widehat{X}_n)) = tr(V_n^{(i)T} A^T \widehat{R}_n), \end{aligned}$$

and thus

$$0 = V_n^T A^T \diamond \widehat{R}_n.$$

Therefore, condition (24) is equivalent to

$$\widehat{R}_n \perp_F AK_n(\widehat{A}, \widehat{R}_0).$$

Note that the Krylov subspace is multiplied with A instead of $\widehat{A}$. Therefore, condition (14) is satisfied. Mathematically, using Theorem 3.2, these conditions give conditions (17) and (18), namely

$$X_n \in X_0 + K_n(\widehat{A}, \widehat{R}_0) + \mathcal{U}, \tag{25}$$

$$R_n = B - AX_n \perp_F AK_n(\widehat{A}, \widehat{R}_0) + A\mathcal{U}, \tag{26}$$

in the sense that

$$X_n = \widetilde{P}_A \widehat{X}_n + Q_A A^T B, \quad \text{and} \quad R_n = \widehat{R}_n. \tag{27}$$

Thus, using a global MR-type method, we can solve deflated matrix equation (23) and apply correction step (27). Then, the obtained solution satisfies conditions (25) and (26).

From relation (24), we have the minimization property

$$\|\widehat{R}_n\|_F = \min_{Z \in K_n(\widehat{A}, \widehat{R}_0)} \|\widehat{R}_0 - \widehat{A}Z\|_F. \tag{28}$$

There are a number of ways to implement global MR-type methods, in each one, a basis of $K_n \equiv K_n(\widehat{A}, \widehat{R}_0)$ is generated and (28) is replaced by an unconstrained n-dimensional least-squares problem. We assume that it successfully generates a basis if and only if $\dim K_n = n$.

Theorem 5.1. *Consider an arbitrary matrix $\widehat{A} \in \mathbb{R}^{m \times m}$ and a matrix $\widehat{B} \in \mathcal{R}(\widehat{A})$ (i.e., the matrix equation $\widehat{A}X = \widehat{B}$ is consistent). Then the following conditions are equivalent:*

(1) *For each initial guess $X_0 \in \mathbb{R}^{m \times s}$ the global MR-type method applied to the matrix equation $\widehat{A}X = \widehat{B}$ is well defined at each iteration step n and it terminates with a solution of the equation.*
(2) $\mathcal{R}(\widehat{A}) \cap \mathcal{N}(\widehat{A}) = 0$.

Proof. We assume that $\mathcal{R}(\widehat{A}) \cap \mathcal{N}(\widehat{A}) \neq 0$, and we will construct an initial guess for which the global MR-type method does not terminate with the solution. For a nonzero matrix $Y \in \mathcal{R}(\widehat{A}) \cap \mathcal{N}(\widehat{A})$ there exists a matrix $\widehat{Y} \in \mathbb{R}^{m \times s}$, such that $Y = \widehat{A}\widehat{Y}$, and since $\widehat{B} = \widehat{A}X$ is consistent, there exists a matrix $\widehat{X} \in \mathbb{R}^{m \times s}$ with $\widehat{B} = \widehat{A}\widehat{X}$. Then the initial guess $X_0 := \widehat{X} - \widehat{Y}$ gives $R_0 = \widehat{B} - \widehat{A}X_0 = \widehat{B} - \widehat{A}\widehat{X} + \widehat{A}\widehat{Y} = Y$. But since $Y \in \mathcal{N}(\widehat{A})$, we obtain $\widehat{A}R_0 = 0$, so the global MR-type method terminates at the first iteration with the approximation X_0, for which $R_0 = Y \neq 0$. Thus, for this particular initial guess X_0, the global MR-type method cannot determine the solution of $\widehat{A}X = \widehat{B}$.

Conversely, it is trivial that $\dim \widehat{A}K_n \leq \dim K_n \leq n$ for each n. Since the matrix equation $\widehat{A}X = \widehat{B}$ is consistent, $\widehat{R}_0 \in \mathcal{R}(\widehat{A})$ and $K_n \subseteq \mathcal{R}(\widehat{A})$ for each n. Condition $\mathcal{R}(\widehat{A}) \cap \mathcal{N}(\widehat{A}) = 0$ implies that $\dim \widehat{A}K_n = \dim K_n$ for each n, thus there cannot be breakdown through rank deficiency of the least-squares problem (28) (which occurs when $\dim \widehat{A}K_n < \dim K_n$). Therefore, the global MR-type method does not break down at the nth step and X_n is uniquely defined. □

In the sense of $\dim \widehat{A}K_n = \dim K_n$, since $\widehat{A}(K_n) \subset K_{n+1}$, we have $\dim \widehat{A}(K_n) \leq \dim K_{n+1} \leq n + 1$. If $\dim K_{n+1} = \dim \widehat{A}(K_n)$, then we must have $\widehat{A}(K_n) = K_{n+1}$, hence $\widehat{R}_0 \in \widehat{A}(K_n)$. It follows from (28) that $\widehat{R}_n = 0$ and $\widehat{A}\widehat{X}_n = \widehat{B}$. In this case, the global

MR-type method determines a solution without breakdown and then breaks down at the next step through degeneracy of the Krylov subspace (which occurs when $\dim K_k < k$).

Corollary 5.2. *Consider the deflated system (23). Then condition 1 in Theorem 5.1 is satisfied if and only if* $\mathfrak{U} \cap (A\mathfrak{U})^{\perp} = 0$. *In particular, the latter condition is satisfied when* $\mathfrak{U}$ *is an exact* A*-invariant subspace, i.e., when* $A\mathfrak{U} = \mathfrak{U}$.

Proof. Using the properties of the projection P_A from Lemma 3.1 and the fact that A is nonsingular, we obtain

$$\mathcal{N}(\widehat{A}) = \mathcal{N}(P_A A) = A^{-1}\mathcal{N}(P_A) = \mathfrak{U},$$
$$\mathcal{R}(\widehat{A}) = \mathcal{R}(P_A A) = \mathcal{R}(P_A) = (A\mathfrak{U})^{\perp}.$$

The result now follows from Theorem 5.1. If $A\mathfrak{U} = \mathfrak{U}$, then $\mathfrak{U} \cap (A\mathfrak{U})^{\perp} = 0$ holds trivially. □

5.1. Deflated and augmented global MINRES method

In this section, we assume that A is symmetric, nonsingular, and possibly indefinite. In this case, the global MR-type method is the global MINRES (Gl-MINRES) method. There are two versions of the MINRES algorithm which are based on efficient three-term recurrences. One is based on Lanczos algorithm and Givens Rotations [11,23] and the other one was presented by Wang [28]. We consider the global variant of Wang and present a deflated and augmented version of this algorithm.

We also consider $\mathcal{B} = A$ and get the following deflated matrix equation

$$\widehat{A}X = \widehat{B}, \tag{29}$$

where $\widehat{A} := P_A A$, $\widehat{B} := P_A B$.

If we start Gl-MINRES with an initial guess X_0 and corresponding initial residual $\widehat{R}_0 = \widehat{B} - \widehat{A}X_0 = P_A(B - AX_0)$ then the iterations $\widehat{X}_n$ and the residuals $\widehat{R}_n$ are characterized by two conditions

$$\widehat{X}_n \in X_0 + K_n(\widehat{A}, \widehat{R}_0), \tag{30}$$
$$\widehat{R}_n = \widehat{B} - \widehat{A}X_n \perp_F \widehat{A}K_n(\widehat{A}, \widehat{R}_0). \tag{31}$$

In general, the deflated matrix $\widehat{A} = P_A A = A - AQ_A A^2$ is not symmetric, even when A is symmetric. Because P_A is a projection, we can show that

$$K_n(P_A A, P_A V) = K_n(P_A A P_A, P_A V)$$

holds for every matrix $V \in \mathbb{R}^{m\times s}$. Clearly, the matrix $P_A A P_A$ is symmetric (since A and P_A are symmetric). Thus, the Krylov subspaces we work with are generated by a symmetric matrix and we can apply the Gl-MINRES method using conditions (30) and (31) for the deflated matrix equation (29). As shown in Section 5, these conditions combined with the final correction (27), give conditions (25) and (26).

When we apply the Gl-MINRES algorithm for the deflated matrix equation (29), we use the following relation

$$\begin{aligned} <\widehat{R}_j, \widehat{A}\widehat{R}_j>_F &= tr(\widehat{R}_j^T \widehat{A}\widehat{R}_j) = tr((B - A\widehat{X}_j)^T P_A^T P_A A\widehat{R}_j) = tr((B - A\widehat{X}_j)^T P_A^T A\widehat{R}_j) \\ &= tr(\widehat{R}_j^T A\widehat{R}_j) = <\widehat{R}_j, A\widehat{R}_j>_F . \end{aligned}$$

We know that in general $\mathcal{R}(A^T) = \mathcal{N}(A)^{\perp}$ for every matrix A. Now, if we can determine the deflated matrix $\widehat{A}$ with property

$$\mathcal{N}(\widehat{A}) = \mathcal{N}(\widehat{A}^T),$$

then $\mathcal{N}(\widehat{A}) = \mathcal{R}(\widehat{A})^{\perp}$ and hence condition 1 in Theorem 5.1 is satisfied. Consequently, if the deflated matrix $\widehat{A}$ is symmetric with a corresponding consistent deflated matrix equation, Gl-MINRES for this matrix equation cannot break down for any initial guess. Using matrices (12), we split the solution X of (1) as

$$X = P_A X + (I - P_A)X = P_A X + AQ_A AX = P_A X + AQ_A B, \tag{32}$$
$$X = \widetilde{P}_A + (I - \widetilde{P}_A)X = \widetilde{P}_A X + Q_A A^2 X = \widetilde{P}_A X + Q_A AB. \tag{33}$$

Using (33), the matrix equation (1) becomes $A(\widetilde{P}_A X + Q_A AB) = B$. From definition P_A and $A\widetilde{P}_A = P_A A$ of Lemma 3.1, we see that this is equivalent to

$$P_A AX = P_A B$$

substitution of (32) in this equation, we obtain $P_A A(P_A X + AQ_A B) = P_A B$ which is equivalent to

$$P_A A P_A X = P_A \widetilde{P}_A^T B. \tag{34}$$

Now, we can show the following result for the Gl-MINRES method applied to symmetric equation (34).

Theorem 5.3. *For each initial matrix $X_0 \in \mathbb{R}^{m\times s}$, the Gl-MINRES method applied to matrix equation (34) gives (in exact arithmetic) well defined iteration $\overline{X}_n$ at each step $n \geq 1$ until it terminates with a solution. Moreover, the sequence of iterations*

$$X_n := \widetilde{P}_A(P_A \overline{X}_n + A Q_A B) + Q_A A B, \tag{35}$$

is well defined. It terminates (in exact arithmetic) with the exact solution X of the original matrix equation $AX = B$ and its residuals are given by $R_n = B - AX_n = P_A \widetilde{P}_A^T B - P_A A P_A \overline{X}_n$.

Proof. Since the matrix equation (34) is a consistent equation with a symmetric matrix $P_A A P_A$, then we can apply Theorem 5.1. Therefore, the Gl-MINRES method applied to the matrix equation (34) cannot break down for any initial guess. Also, the nth residual of the original matrix equation $AX = B$ is given by

$$\begin{aligned} R_n &= B - AX_n = B - A(\widetilde{P}_A(P_A \overline{X}_n + A Q_A B) + Q_A A B) \\ &= B - A\widetilde{P}_A(P_A \overline{X}_n + A Q_A B) - A Q_A A B \\ &= (I - A Q_A A)B - P_A A(P_A \overline{X}_n + A Q_A B) \\ &= P_A B - P_A A P_A \overline{X}_n - P_A A^2 Q_A B \\ &= P_A(I - A^2 Q_A)B - P_A A P_A \overline{X}_n \\ &= P_A \widetilde{P}_A^T B - P_A A P_A \overline{X}_n. \end{aligned} \tag{36}$$

We see that R_n is equal to the nth Gl-MINRES residual for equation (34). In particular, this implies that the exact solution of matrix equation (1) is given by (35) when a solution $\overline{X}_n$ of (34) is determined by Gl-MINRES. □

6. Numerical results

In this section, we present numerical examples to illustrate the effectiveness of Algorithm 1 to solve matrix equations (1). Note that we can consider different versions of Algorithm 1 that depend on the properties of the matrix A.

Examples are carried out using double precision floating point arithmetic in MATLAB 7.12.0. All test matrices are taken from the Matrix Market [17] with the exception of Example 6.4. Since eigenvalues of the operator close to zero decelerate the convergence of the Krylov subspace methods, we first compute (by the MATLAB code eigs$(A, k, 'sm')$ for sparse matrices with accuracy 10^{-16}) the k smallest magnitude eigenvalues of A and their corresponding eigenvectors denoted by $U_1, U_2, \ldots, U_k$. Then we apply Algorithm 1 with $U = [U_1, U_2, \ldots, U_k]$. Also, the iterations are started with $\widehat{X}_0 = 0$. Also, we give the CPU-time (that includes CPU-time for computation of eigs) for each algorithm in parenthesis and we denote the size of the matrix A with m. Tolerance of computed eigenvectors by eigs in all examples is given 10^{-16} except Example 6.5.

Example 6.1. In this example, we use matrices NOS5, GR-30-30 and BCSSTK06 and compare the performance of the Gl-CG [25] and Def-Aug-Gl-CG algorithms. We consider the 10 smallest eigenvalues of these matrices. The right-hand side B is chosen such that the exact solution X is a matrix of order $m \times s$ whose ith column has all entries equal to one except the ith entry which is zero. The stopping criterion is

$$\max_{1\leq i\leq s} \frac{\|b^{(i)} - Ax^{(i)}\|_2}{\|B\|_F} < 10^{-7},$$

where $b^{(i)}$ and $x^{(i)}$ for $i = 1, 2, \ldots, s$ are columns in the matrices B and X, respectively.

The numerical results are shown in Table 1. This table shows that the Def-Aug-Gl-CG algorithm converges faster than Gl-CG by considering the corresponding eigenvectors of the 10 smallest eigenvalues for columns of matrix U. Also from Table 1, we see that for the Gl-CG and the Def-Aug-Gl-CG algorithms, the choice $s = 2$ is less cost effective than $s = 4$.

Fig. 1 shows the results obtained with Gl-CG and the Def-Aug-Gl-CG for matrices NOS5 and GR-30-30 with $s = 4$ and $k = 10$. As seen from this figure, the Def-Aug-Gl-CG method converges faster and gives a much smoother convergence behavior than Gl-CG.

Example 6.2. In this example, we compare the performance of the Gl-MINRES and the Def-Aug-Gl-MINRES algorithms for the symmetric matrices BLCKHOLE, JAGMESH2 and JAGMESH4. We consider the 10 and 15 smallest magnitude eigenvalues of these matrices. Let $B = rand(m, s)$ and the stopping criterion is

$$\frac{\|R_j\|_F}{\|B\|_F} < 10^{-7}.$$

Table 1
Numerical results of Gl-CG and Def-Aug-Gl-CG.

Matrix	m	k	Method	$s=2$	$s=4$
NOS5	468	10	Def-Aug-Gl-CG	143 (0.42)	143 (0.48)
			Gl-CG	336 (0.50)	365 (1.37)
GR-30-30	900	10	Def-Aug-Gl-CG	28 (0.35)	28 (0.41)
			Gl-CG	52 (0.44)	52 (0.44)
BCSSTK06	420	10	Def-Aug-Gl-CG	1006 (1.87)	1006 (2.19)
			Gl-CG	2397 (3.35)	1766 (4.84)

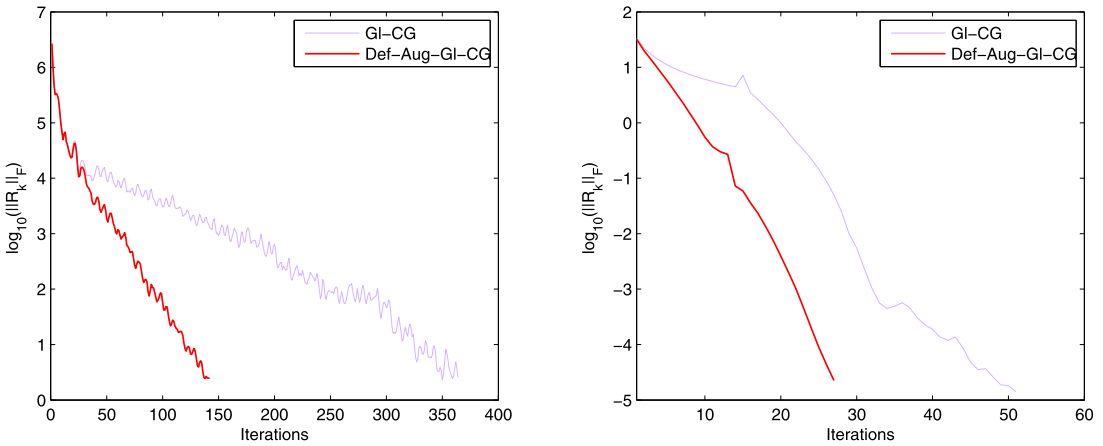

Fig. 1. The convergence history for NOS5 (on the left) and GR-30-30 (on the right).

Table 2
Numerical results of Gl-MINRES and Def-Aug-Gl-MINRES.

Matrix	m	k	Method	$s=2$	$s=4$
JAGMESH2	1009	15	Def-Aug-Gl-MINRES	877 (0.52)	889 (0.64)
		10	Def-Aug-Gl-MINRES	1106 (0.62)	1140 (0.80)
			Gl-MINRES	1741 (0.82)	1771 (1.03)
JAGMESH4	1440	15	Def-Aug-Gl-MINRES	1144 (0.82)	1156 (0.93)
		10	Def-Aug-Gl-MINRES	1543 (0.90)	1556 (1.14)
			Gl-MINRES	2531 (1.30)	2535 (1.91)
BLCKHOLE	2132	15	Def-Aug-Gl-MINRES	2350 (1.71)	2357 (2.54)
		10	Def-Aug-Gl-MINRES	3284 (2.39)	3284 (3.34)
			Gl-MINRES	4866 (2.89)	5030 (4.16)

As seen from Table 2, the Def-Aug-Gl-MINRES method requires less iteration steps and CPU-time than Gl-MINRES. Also, Def-Aug-Gl-MINRES is more effective for $k=15$ than for $k=10$. Table 2 shows that Def-Aug-Gl-MINRES and Gl-MINRES algorithms become expensive as s increases.

Fig. 2 shows that for $s=4$ and $k=15$, the Def-Aug-Gl-MINRES for matrices JAGMESH2 and BLCKHOLE gives a much smoother convergence behavior than Gl-MINRES.

Example 6.3. In this example, we use matrices SHERMAN1, SHERMAN4 and CAVITY01 and compare the performance of the Gl-GMRES(25) and the Def-Aug-Gl-GMRES(25) algorithms. We consider the 10 smallest eigenvalues of these matrices and let $B = rand(m, s)$. The stopping criterion is

$$\frac{\|R_j\|_F}{\|B\|_F} < 10^{-7}.$$

Also, we compare the Def-Aug-Gl-GMRES(25) and Def-Aug-Gl-GMRES(50) algorithms.

In Table 3, we observe that the iteration steps and CPU-time for Def-Aug-Gl-GMRES(25) are better than Gl-GMRES(25). As shown in Table 4, the Def-Aug-Gl-GMRES(50) algorithm requires less iteration steps and more CPU-time than Def-Aug-Gl-GMRES(25). The results obtained in Tables 3 and 4 show the effectiveness of the choice $s=2$.

Fig. 3 shows the results obtained with Gl-GMRES(25) and Def-Aug-Gl-GMRES(25) for matrices CAVITY01 and SHERMAN1 for $s=2$ and $k=10$. As seen from this figure, Def-Aug-Gl-GMRES(25) converges faster than Gl-GMRES(25).

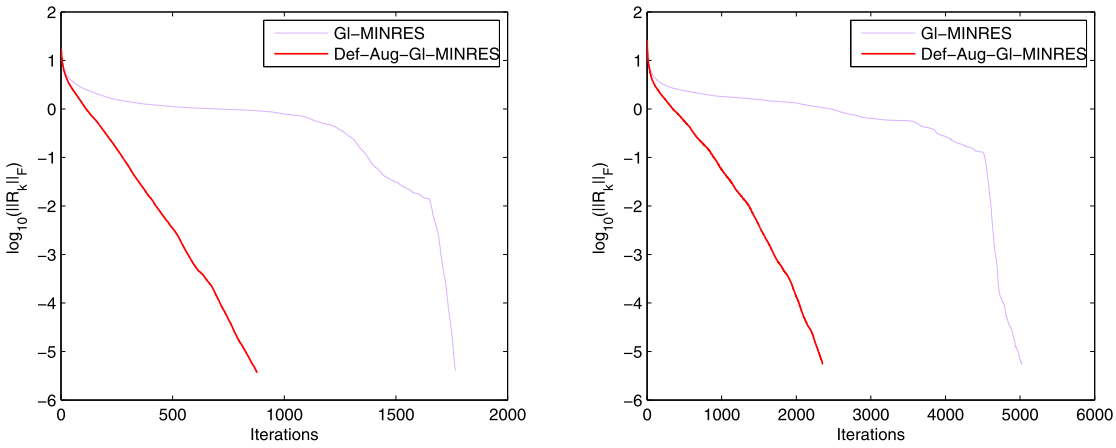

Fig. 2. The convergence history for JAGMESH2 (on the left) and BLCKHOLE (on the right).

Table 3
Numerical results of Gl-GMRES(25) and Def-Aug-Gl-GMRES(25).

Matrix	m	k	Method	$s=2$	$s=4$
CAVITY01	317	10	Def-Aug-Gl-GMRES(25)	20 (0.89)	21 (0.95)
			Gl-GMRES(25)	135 (4.65)	155 (5.16)
SHERMAN1	1000	10	Def-Aug-Gl-GMRES(25)	19 (4.10)	20 (4.50)
			Gl-GMRES(25)	164 (6.12)	165 (7.87)
SHERMAN4	1104	10	Def-Aug-Gl-GMRES(25)	3 (0.90)	3 (0.91)
			Gl-GMRES(25)	28 (1.11)	29 (1.48)

Table 4
Numerical results of Def-Aug-Gl-GMRES(25) and Def-Aug-Gl-GMRES(50).

Matrix	m	k	Method	$s=2$	$s=4$
CAVITY01	317	10	Def-Aug-Gl-GMRES(25)	20 (0.89)	21 (0.95)
			Def-Aug-Gl-GMRES(50)	5 (1.00)	5 (1.00)
SHERMAN4	1104	10	Def-Aug-Gl-GMRES(25)	3 (0.90)	3 (0.91)
			Def-Aug-Gl-GMRES(50)	2 (1.30)	2 (1.32)

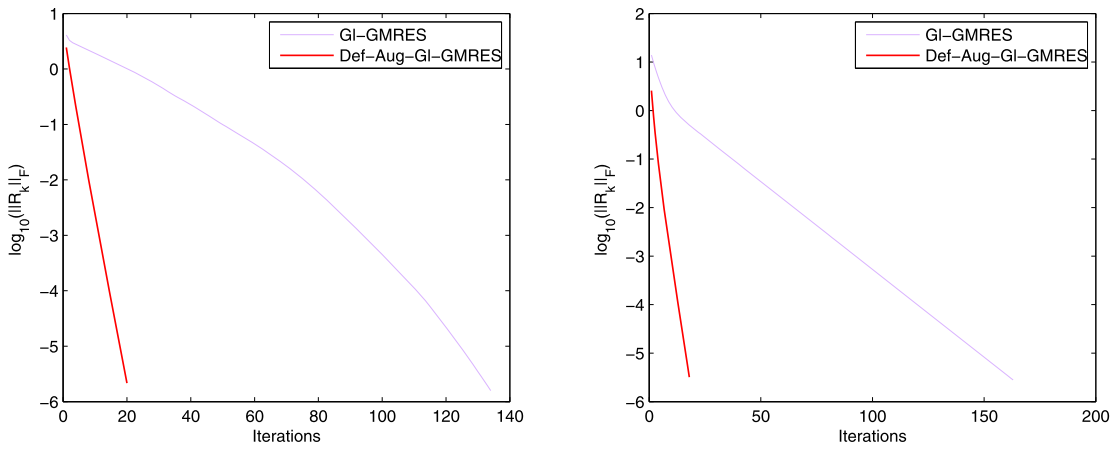

Fig. 3. The convergence history for CAVITY01 (on the left) and SHERMAN1 (on the right).

Table 5
Numerical results of Example 6.4 for $n_1 = 30$, $p_1 = 5$, $p_2 = 10$ and $p_3 = 20$.

Matrix	k	Method	$s = 10$	$s = 20$	$s = 30$
A	10	Def-Aug-Gl-GMRES(25)	3 (0.76)	3 (0.98)	3 (1.37)
		Gl-GMRES(25)	7 (0.56)	7 (1.07)	7 (1.47)
A	20	Def-Aug-Gl-GMRES(25)	2 (0.54)	2 (0.72)	2 (0.93)
		Gl-GMRES(25)	7 (0.56)	7 (1.07)	7 (1.47)

Table 6
Numerical results of Def-Aug-Gl-GMRES(25) with $s = 2$.

Matrix	k	Tolerance of eigenvectors	Iteration	Residual norm
CAVITY01	15	10^{-16}	11 (0.48)	2.1495×10^{-6}
		10^{-5}	12 (0.49)	1.6012×10^{-6}
CAVITY01	20	10^{-16}	12 (0.52)	1.6795×10^{-6}
		10^{-4}	13 (0.54)	2.3249×10^{-6}

Example 6.4. In this example, we consider constant convection-diffusion partial differential operator [33]

$$-\Delta u(x, y) + 2p_1 u_x(x, y) + 2p_2 u_y(x, y) - p_3 u(x, y) = \lambda u(x, y)$$

on a square region $[0, 1] \times [0, 1]$ with the boundary condition $u(x, y) = 0$, where p_1, p_2 and p_3 are positive constant. Discretizing by five differences on uniform $n_1 \times n_1$ grid points using the row wise natural ordering gives rise to a block tridiagonal matrix A for order $m = n_1^2$. Therefore we get

$$A = \begin{pmatrix} T & (\beta+1)I & & & \\ (-\beta+1)I & T & (\beta+1)I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & (\beta+1)I \\ & & & (-\beta+1)I & T \end{pmatrix},$$

where

$$T = \begin{pmatrix} 4-\theta & \gamma-1 & & & \\ -\gamma-1 & 4-\theta & \gamma-1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \gamma-1 \\ & & & -\gamma-1 & 4-\theta \end{pmatrix},$$

and $\beta = p_1 h$, $\gamma = p_2 h$, $\theta = p_3 h^2$ and $h = \frac{1}{n_1+1}$.

We let $B = rand(m, s)$ and the stopping criterion is

$$\frac{\|R_j\|_F}{\|B\|_F} < 10^{-7}.$$

Table 5 shows that the number of iterations and CPU-time for Def-Aug-Gl-GMRES(25) are better than Gl-GMRES(25) as s increases. Also, Def-Aug-Gl-GMRES(25), for choice $k = 20$ is faster than $k = 10$.

Example 6.5. In this example, we consider matrix CAVITY01 and compare the performance of Def-Aug-Gl-GMRES(25) algorithm with computed eigenvectors by eigs with different accuracies. The right-hand side B is chosen such that the exact solution X is a matrix of order $m \times s$ whose ith column has all entries equal to one except the ith entry which is zero. The stopping criterion is

$$\frac{\|R_j\|_F}{\|B\|_F} \leq 10^{-7}.$$

Table 6, shows that the number of iterations, CPU-time and residual norm in Def-Aug-Gl-GMRES(25) algorithm depend on the accuracy of computed eigenvectors by eigs.

7. Conclusions

In this paper, to accelerate the convergence of global Krylov subspace methods, we presented a framework for deflated and augmented global methods and present the algorithm of this method. Therefore, we theoretically analyzed versions of this method for the global OR-type methods and the global MR-type methods. Also, for symmetric matrices, we presented deflated and augmented Gl-MINRES which uses a symmetric deflated matrix and without breakdown gives (in exact arithmetic) the exact solution of the matrix equation (1). In Example 6.5, we compared the performance of Def-Aug-Gl-GMRES(25) algorithm with computed eigenvectors by eigs in Matlab with different accuracies. Finally, our numerical experiments illustrate the effectiveness of different versions of the new algorithm.

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