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The deflated flexible GMRES with an approximate inverse preconditioner

by

Takuro Kutsukake
Takashi Nodera

Takuro Kutsukake
School of Fundamental Science and Technology
Keio University

Takashi Nodera
Department of Mathematics
Keio University

Department of Mathematics
Faculty of Science and Technology
Keio University

3-14-1 Hiyoshi, Kohoku-ku, Yokohama, 223-8522 Japan

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Takuro KUTSUKAKE[1] Takashi NODERA[2]

Abstract

This is a study of a preconditioning technique, based on an approximate inverse, which can be considered to be a type of a flexible GMRES (FGMRES). The FGMRES plays an important role in modern iterative solvers for large sparse nonsymmetric linear systems of equations. Morgan [SIAM J. Sci. Comput., Vol. 24, pp. 20–37, 2002] developed a new method that deflates the smallest eigenvalues and improves eigenvalue distribution. Several preconditioning methods have been exploited in numerous papers. This study explores a new deflated FGMRES which uses an approximate inverse preconditioner. The results of the numerical experiments for test matrices were tabulated to show that this approach was effective and robust in solving a wide range of problems.

key words. GMRES, Deflation, approximate inverse, Sherman-Morrison Formula
AMS(MOS) subject classifications. 65F10, 65K10

Contents

1 Introduction

For solving a large sparse nonsymmetric linear system of equations:

$$A\boldsymbol{x} = \boldsymbol{b}, \quad \boldsymbol{x} \in R^n. \tag{1}$$

The GMRES [13] is now a standard Krylov subspace iterative method. The GMRES uses the Arnoldi process to build an orthonormal basis for a Krylov subspace given by:

$$\mathcal{K}_m(A, \boldsymbol{r}_0) = \text{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{m-1}\boldsymbol{r}_0\}, \tag{2}$$

where $\boldsymbol{r}_0$ $(= \boldsymbol{b} - A\boldsymbol{x}_0)$ is a initial residual vector, and $\boldsymbol{x}_0$ is an initial guess to the solution of equation (1). If exact arithmetic is used, the GMRES will converge at most n iterations. Since the GMRES is expensive both in terms of computation and in its memory requirements, a restart version is often used, in which a Krylov subspace is restricted to be a fixed dimension m. The Arnoldi process is restarted using the last iterate x_m as a new initial approximation for a restart. Unfortunately, it can be very difficult to select m a priori. If too small a value is selected, its convergence may stall. It is known that a small eigenvalue of A slows down the convergence. Several adaptive techniques of the restart were developed in a number of papers [15, 8, 17]. Recent works on the convergence behavior of the GMRES relates to the superlinear convergence of Ritz values [16]. Basically, convergence occurs as if at each iteration of the GMRES the next smallest eigenvalue in the magnitude is removed from the system of linear equation. Unfortunately, if the GMRES(m) is used, the information of the smallest eigenvalues and corresponding eigenvectors are lost at each restart and as a result, the superlinear convergence may be lost. For this reason, different methods of reducing the negative effects of a restart were explored.

Recently, several schemes that improve the convergence of the GMRES(m) were developed successfully. One of the new techniques explored in this paper employs deflation [6, 3, 4]. This method uses eigenvalues information at the restart mainly to improve the convergence of the GMRES(m). Deflation is defined as when an invariant subspace corresponding to the smallest eigenvalues is approximated, and the influence on the component of the residual vector is eliminated.

This new proposal is a modification of techniques derived from the Deflated FGMRES [2] and Deflated GMRES(m, k, l) [8, 14]. This new algorithm is referred to as the Deflated FGMRES with an approximate inverse of the Sherman-Morrison formula (AISM) preconditioner.

In section 2, the Deflated GMRES is explored briefly. In section 3, the approximate inverse preconditioner which is based on the Sherman-Morrison formula is discussed. In section 4, a new deflated FGMRES with an AISM preconditioner is explored. In section 5, the results of numerical experiments for the test matrices are tabulated. The conclusion follows.

2 Deflated GMRES(m, k)

Morgan [6] developed the Deflated GMRES(m, k) in 2002. The Deflated GMRES(m, k) is normally used to solve large sparse nonsymmetric linear systems [6, 3, 4, 7]. The Deflated GMRES has two parameters m and k, where m is the maximum dimension of the subspace

Algorithm 1 GMRES-DR(m, k)

1: Input: a coefficient matrix A
2: Select an initial guess $\boldsymbol{x}_0$, parameter m and k
3: set $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ and $\beta = \|\boldsymbol{r}_0\|$
4: $\boldsymbol{v_1} = \boldsymbol{r}_0/\|\boldsymbol{r}_0\|$
5: Generate V_m and $\overline{H}_m$ with Arnoldi method
6: Solve $\min\|\boldsymbol{c} - \overline{H}_m\boldsymbol{y}\|$ for $\boldsymbol{y}_m$, where $\boldsymbol{c} = \beta\ \boldsymbol{e}_1$
7: $\boldsymbol{x}_m = \boldsymbol{x}_0 + V_n\boldsymbol{y}_m$, $\boldsymbol{r}_m = \boldsymbol{b} - A\boldsymbol{x}_m$
8: Compute the k smallest eigenpairs $(\tilde{\theta}_i,\tilde{\boldsymbol{g}}_i)$ of $H_m + \beta^2\, H_m^{-T}\boldsymbol{e}_m\boldsymbol{e}_m^T$
9: Set Q_{k+1} from $G_k = [\boldsymbol{g}_1\ \boldsymbol{g}_2\ \ldots\ \boldsymbol{g}_k]$
10: Set $V_{k+1}^{\text{new}} = V_{k+1}Q_{k+1}$ and $\overline{H}_k^{\text{new}} = Q_{k+1}^H\overline{H}_mQ_k$
11: Extend V_{k+1}^{new} and $\overline{H}_k^{\text{new}}$ to V_{m+1} and $\overline{H}_m$ with Arnoldi method
12: **if** $\|\boldsymbol{r}_m\| < tol$ **then**
13: stop iteration
14: **end if**
15: set $\boldsymbol{x}_0 = \boldsymbol{x}_m$
16: Go to line 3

and k is the number of eigenvectors used at the restart. Firstly, V_m and H_m are computed in the same manner as the GMRES(m). Then, let $(\theta_i, \boldsymbol{g}_i)$ be the harmonic Ritz pairs. These are the pairs of eigenvalues and eigenvectors of matrix $H_m + \beta^2 H_m^{-T}\boldsymbol{e}_m\boldsymbol{e}_m^T$, where $\beta = \|\boldsymbol{r}_0\|$ and $\boldsymbol{e}_m$ is a vector where the m-th element is 1 and the other is 0. The next step was to select k eigenvectors corresponding to the k smallest eigenvalues. Here, we have an m harmonic Ritz pair and the eigenvalues $\theta_1, \ldots, \theta_k$ ($\theta_1 \leq \theta_2 \leq \cdots \leq \theta_k$), and the corresponding eigenvectors $\boldsymbol{g}_1, \boldsymbol{g}_2, \ldots, \boldsymbol{g}_k$ are selected. Let G_k be a matrix such that:

$$G_k = (\boldsymbol{g}_1, \boldsymbol{g}_2, \ldots, \boldsymbol{g}_k), \tag{3}$$

and generating G_{k+1} such that,

$$G_{k+1} = \left(\begin{pmatrix} G_k \\ 0_{1\times k} \end{pmatrix}, \boldsymbol{c} - \overline{H}_m\boldsymbol{y} \right). \tag{4}$$

Using Q_{k+1} by QR factorization, V_{k+1} and H_k are generated, where V_{k+1} is n by $k+1$ matrix and H_k is k by k matrix. They are not large enough to be used in the least squares method. Therefore, it becomes necessary to extend V_{k+1} and H_k to V_m and H_m by the Arnoldi method that starts at the $k+1$-th iteration. This method is called the GMRES-DR(m, k), which is shown in Algorithm 1.

2.1 AISM preconditioner

Preconditioner M can reduce the number of iterations, because the properties of the matrix is improved by preconditioning. Right preconditioning is done through multiplying M from the right of A in the left hand side of equation (5) such that:

$$\begin{aligned} AM\boldsymbol{y} &= \boldsymbol{b}, \\ \boldsymbol{x} &= M\boldsymbol{y}. \end{aligned} \tag{5}$$

Algorithm 2 Approximate Inverse based on Sherman-Morrison formula (AISM)

Input a matix $A = [\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n]$ and a parameter s
for $k = 1 : n$ **do**
  Set $\boldsymbol{x}_k = \boldsymbol{e}_k, \quad \boldsymbol{y}_k = (\boldsymbol{a}_k - s\,\boldsymbol{e}_k)^T$
  $\boldsymbol{u}_k = \boldsymbol{x}_k$
  $\boldsymbol{v}_k = \boldsymbol{y}_k$
  for $i = 1 : k-1$ **do**
    $\boldsymbol{u}_k = \boldsymbol{u}_k - \dfrac{(\boldsymbol{v}_i)_k}{s\,r_i}\,\boldsymbol{u}_i;$
    $\boldsymbol{v}_k = \boldsymbol{v}_k - \dfrac{\boldsymbol{y_k}^T\boldsymbol{u}_i}{s\,r_i}\,\boldsymbol{v}_i;$
  end for
  for $i = 1 : n$ **do**
    if$|(\boldsymbol{u}_k)_i| < tolU$ dropoff $(\boldsymbol{u}_k)_i$
    if$|(\boldsymbol{v}_k)_i| < tolV$ dropoff $(\boldsymbol{v}_k)_i$
  end for
  $\boldsymbol{r}_k = 1 + (\boldsymbol{v}_k)_k/s$
end for
Define U, V and $\Omega = \mathrm{diag}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n)$
Set $M = s^{-1}\,I_n - s^{-2}\,U\Omega^{-1}V^T$

In general, the preconditioning matrix is often chosen such that $AM = I_n$ where I_n is the identity matrix. In other words, M will be selected to $M \approx A^{-1}$. Therefore, an approximate inverse matrix of A is often calculated and used as a right preconditioning matrix M. One way of calculating an approximate inverse matrix is by using the Sherman-Morrison formula [1]. This method called the Approximate Inverse based on the Sherman-Morrison formula, will be referred to as the AISM method from hereforth. In Algorithm 2, the AISM method was used for computing an approximate inverse matrix. An efficient parallel implementation of this method was given in papers [10, 18]. In this scenario, s was a parameter of a scalar and often used as $s = 1.5\|A\|_\infty$ ([1, 10, 18]). The non-zero elements were dropped off by the threshold value *tol* for keeping U and V a sparse matrix. By dropping off the non-zero elements, both computation costs and memory requirements were saved. Through the AISM method, the approximate inverse matrix M was obtained such that:

$$A^{-1} \approx s^{-1}I_n - s^{-2}U\Omega^{-1}V^T, \tag{6}$$

where $\Omega = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

3 Deflated FGMRES

The Deflated FGMRES was first proposed by Giraud et al. [2]. Please refer to this paper for additional details. If preconditioner M is an approximate inverse matrix of A, then the preconditioned matrix AM is clearly close to identity matrix I_n. Because all the eigenvalues of the identity matrix is 1, it is thought that most eigenvalues of AM gather around 1. Please see Figure 1 for further details. The eigenvalue distribution of the original matrix A

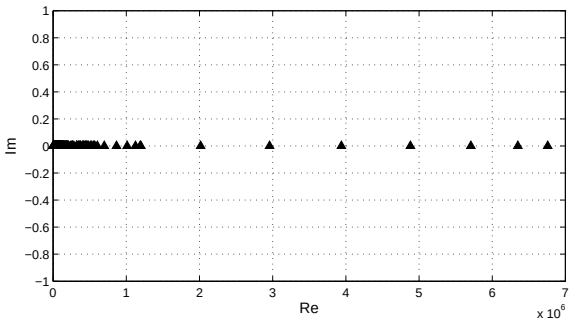

Figure 1: Sherman3 - Distribution of eigenvalues of original coefficient matrix A

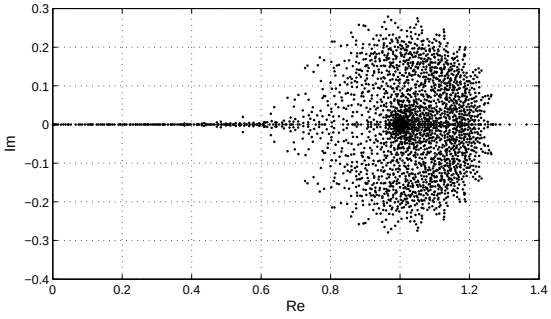

Figure 2: Sherman3 - Distribution of eigenvalues of AM using AISM preconditioner

named sherman3 was obtained from the Matrix Market [5]. Figure 2 shows the eigenvalue distribution of the preconditioned matrix AM. In Figure 2, eigenvalues were close to 1. Focusing on this point, in the deflation method, the eigenvalues away from the cluster were selected, instead of the smallest eigenvalues.

The deflation method retains the k eigenvectors associated with eigenvalues such as $|1 - \lambda_i|$ of the largest magnitude. With this choice, eigenvalues located away from a cluster around the eigenvalue of the perfect preconditioned operator AM with $M = A^{-1}$ were targeted. This possibly allowed the simultaneous deflation of eigenvalues of both the smallest and largest magnitude. This method is called the GMRES-DRC. In general, the GMRES-DRC needs another preconditioner, because numerous eigenvalues must be clustered around 1, applying good preconditioning techniques. For efficient preconditioning, the aforementioned AISM method can be applied. The Flexible GMRES-DRC with an AISM preconditioner is given in Algorithm 3.

4 Numerical experiments

In this section, numerical results will be presented comparing the two methods described in the previous sections on the two test problems. All computations of the numerical experiments were done on a PC with 2.93GHz and an 8 Gbyte main memory using MATLAB R2012b. These results were tabulated to illustrate the efficiency of the proposed method.

In these experiments, $\boldsymbol{x}_0 = 0$ for an initial approximate solution, and a solution $\boldsymbol{x}_i$ is considered to be converged if the residual norm satisfies the following convergence criterion:

$$\|\boldsymbol{r_i}\|_2/\|\boldsymbol{b}\|_2 < 1.0 \times 10^{-12}, \tag{7}$$

where $\boldsymbol{r}_i$ is the residual vector of the i-th iteration.

4.1 Example 1

For the first example, matrix Sherman3 [5] taken from an oil reservoir simulation was used. It was 5005 by 5005 and had 20033 non-zero elements and its condition number was 6.90×10^{16}. In producing an approximate inverse matrix through the AISM method, the

Algorithm 3 Flexible GMRES-DRC(m, k) with AISM preconditioner

1: Input: a coefficient matrix A
2: Select an initial guess $\boldsymbol{x}_0$, parameter m and k
3: Compute preconditioner M with AISM method
4: set $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ and $\beta = \|\boldsymbol{r}_0\|$
5: $\boldsymbol{v}_1 = \boldsymbol{r}_0/\|\boldsymbol{r}_0\|$
6: Generate V_m and $\overline{H}_m$ with Flexible Arnoldi method
7: Solve $\min\|\boldsymbol{c} - \overline{H}_m\boldsymbol{y}\|$ for $\boldsymbol{y}_m$, where $\boldsymbol{c} = \beta\,\boldsymbol{e}_1$
8: $\boldsymbol{x}_m = \boldsymbol{x}_0 + V_n\boldsymbol{y}_m$, $\boldsymbol{r}_m = \boldsymbol{b} - A\boldsymbol{x}_m$
9: Compute the k eigenpairs away from Cluster $(\tilde{\theta}_i, \tilde{\boldsymbol{g}}_{\boldsymbol{i}})$ of $H_m + \beta^2\, H_m^{-T}\boldsymbol{e}_m\boldsymbol{e}_m^T$
10: Set Q_{k+1} from $G_k = [\boldsymbol{g}_1, \boldsymbol{g}_2, \ldots, \boldsymbol{g}_k]$
11: Set $V_{k+1}^{\text{new}} = V_{k+1}Q_{k+1}$ and $\overline{H}_k^{\text{new}} = Q_{k+1}^H\overline{H}_mQ_k$
12: Extend V_{k+1}^{new} and $\overline{H}_k^{\text{new}}$ to V_{m+1} and $\overline{H}_m$ with Arnoldi method
13: **if** $\|\boldsymbol{r}_m\| < tol$ **then**
14: stop iteration
15: **end if**
16: set $\boldsymbol{x}_0 = \boldsymbol{x}_m$
17: Go to line 4

Table 1: Example 1 - Nonzero elements and computation time for AISM

	AIMS preconditioner			FGMRES		
tol	nnz$U$	nnz$V$	time (sec)	iter	time (sec)	Tct (sec)
–	3167626	4178274	62.0	—	—	—
0.001	1304243	3183793	39.7	3	0.5	40.2
0.010	205002	2321427	26.8	5	0.7	27.5
0.100	20890	1142553	20.8	30	1.6	22.4
0.200	11184	775633	2.1	57	20.4	22.5
0.500	6574	584420	2.1	74	18.8	20.9
1.000	5005	517114	18.1	—	—	—

threshold parameter *tol* was changed by dropping off the non zero elements of matrices U and V, and the effect on the convergence of residual norms in Table 1 were observed. In this table, "—" indicates that dropping off should not be implemented, and time(sec) is necessary to produce an approximate inverse matrix by the AISM method. Both nnz$U$ and nnz$V$ indicate the number of non-zero element of matrices U and V, and time(sec) is the computation time for arriving at the approximate solution without producing a preconditioning matrix. Iter refers to the iteration numbers of algorithms, and "—" shows that the algorithm was not able to converge. It can be seen that the total computation time (Tct) for $tol = 0.5$ was the smallest. Figure 3 shows a comparison of the iteration numbers for FGMRES(m), FGMRES-DR(m, k) and FGMRES-DRC(m, k). The AISM preconditioner with parameter $tol = 0.5$ was used. In Figure 3, it can be seen that the iteration number of FGMRES-DRC(m, k) with the AISM preconditioner was the smallest.

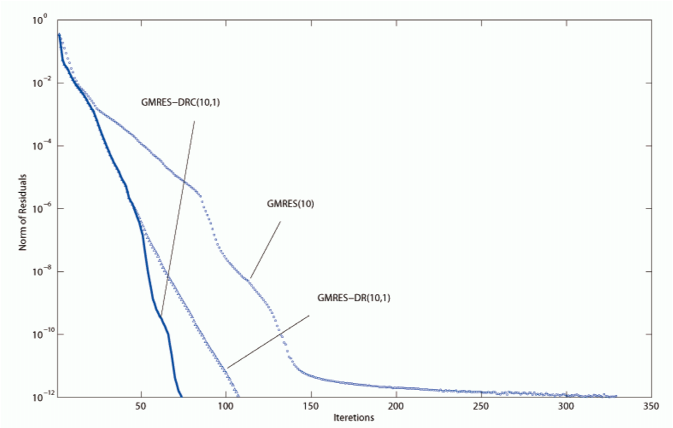

Figure 3: Example 1 - The behavior of residual norms vs iterations for each Deflated FGMRES

Table 2: Example 2 - Iterations and Computation Time (sec) for the Deflated FGMRES with preconditioner

method	preconditioner					
	none		ILU(1)		AISM	
	iter	time (sec)	iter	time (sec)	iter	time (sec)
FGMRES(10)	14266	73.9	3167	72.3	1644	19.9
FGMRES-DR(10,1)	15927	156.8	345	7.6	192	3.0
FGMRES-DRC(10,1)	17201	168.8	835	17.1	165	2.6

4.2 Example 2

The second example is the Sherman5, which is an oil reservoir simulation challenge matrix from the Matrix Market (Harwell-Boeing Collection) [5]. This problem has a 3312×3312 real nonsymmetric matrix and the condition number is 3.9×10^5. Figure 4 shows the distribution of eigenvalues of the original matrix A. The distribution of eigenvalues of a preconditioned matrix AM is also displayed in Figure 5. It presents both positive and negative separated real eigenvalues and a cluster of eigenvalues around $(1,\ 0)$. Table 2 compares the number of successful convergence cases for the different preconditioners allowed. Two preconditioners are employed. Overall, it was observed that the Deflated FGMRES-DRC$(10, 1)$ with the AISM preconditioner converged significantly faster than other FGMRES solvers.

5 Conclusion

The development of efficient and reliable approximate inverse preconditioners is important for the successful application of scientific computation for solving large and sparse sets of linear systems of equations.

Numerical experiments show that the proposed method, FGMRES-DRC, reduced the

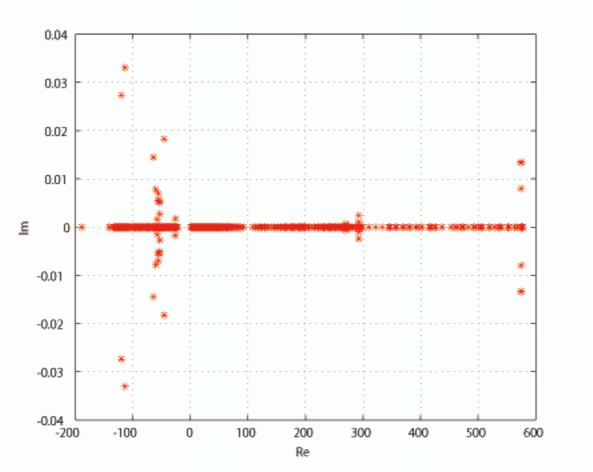

Figure 4: Example 2 - Distribution of the eigenvalues of the original coefficient matrix A

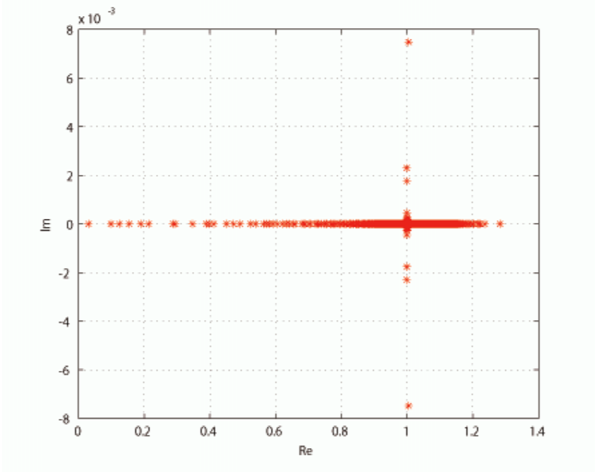

Figure 5: Example 2 - Distribution of the eigenvalues of AM using the AISM preconditioner

numbers of iterations and sped up the convergence of the residual. However, it should be noted that a heuristic estimate of most parameters of the Flexible GMRES-DRC are needed.

Future work is necessary to obtain more experimental results which can find a solution for possibly selecting these appropriate parameters automatically.

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Author addresses

1. **Takuro KUTSUKAKE**, School of Fundamental Science and Technology,Graduate School of Science and Technology, Keio University, JAPAN.
`mailto:kutsukake.takurou@a2.keio.jp`

2. **Takashi NODERA**, Department of Mathematics, Faculty of Science and Technology, Keio University, JAPAN.
`mailto:nodera@math.keio.ac.jp`

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Department of Mathematics
Faculty of Science and Technology
Keio University

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