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KRYLOV SUBSPACE METHODS WITH DEFLATION AND BALANCING PRECONDITIONERS FOR LEAST SQUARES PROBLEMS

Liang Zhao[1], Tingzhu Huang[1,†] and Liangjian Deng[1,†]

Abstract For solving least squares problems, the CGLS method is a typical method in the point of view of iterative methods. When the least squares problems are ill-conditioned, the convergence behavior of the CGLS method will present a deteriorated result. We expect to select other iterative Krylov subspace methods to overcome the disadvantage of CGLS. Here the GMRES method is a suitable algorithm for the reason that it is derived from the minimal residual norm approach, which coincides with least squares problems. Ken Hayami proposed BAGMRES for solving least squares problems in [*GMRES Methods for Least Squares Problems, SIAM J. Matrix Anal. Appl., 31(2010)*, pp.2400-2430]. The deflation and balancing preconditioners can optimize the convergence rate through modulating spectral distribution. Hence, in this paper we utilize preconditioned iterative Krylov subspace methods with deflation and balancing preconditioners in order to solve ill-conditioned least squares problems. Numerical experiments show that the methods proposed in this paper are better than the CGLS method.

Keywords Least squares problems, Krylov subspace methods, deflation preconditioner, GMRES methods, CGLS methods.

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1. Introduction

We assume that the least squares problem is in this form

$$\min_x \|b - Ax\|_2, \tag{1.1}$$

where the coefficient matrix A is large and sparse, and we consider that A is of size $m \times n$, with full column rank and $m \geq n$. When $m = n$, the least squares problems could be regarded as a square case and we can choose typical iterative Krylov methods [7, 18, 19, 21], such as GMRES [21] and Bi-CG [7], to get an approximate solution of the linear system $Ax = b$, minimizing residual under 2-norm. Especially,

†The corresponding author. Email address: tingzhuhuang@126.com (T. Huang), liangjian1987112@126.com (L. Deng)
[1]School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu, Sichuan, 611731, China
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this linear system actually has been applied to many practical applications, such as signal processing [24, 25], image restoration [3, 8, 26–28]. In this paper, we just consider the situation that $m > n$. The least square problem (1.1) is mathematically equivalent to a linear system as this form

$$A^T Ax = A^T b, \tag{1.2}$$

which simply translates the original least squares problems into a square case by premultiplying A^T on two sides of the equal sign. And the system matrix of (1.2) is symmetric positive definite (SPD) so that it could be solved by CG method. That is the strategy of CGLS [1].

However, the condition number of the SPD linear system, in (1.2), influences the convergence of conjugate gradient methods significantly. Notice the following theorem describing the relationship between the condition number of system matrix and the convergence of CG method. (See [20] for illustration)

Theorem 1.1. *Let x_m be the approximate solution obtained at the mth step of the CG algorithm and x_* be the exact solution. $A^T A$ is symmetric positive definite. Then*

$$\|x_* - x_m\|_{A^T A} \leq 2\left(\frac{\sqrt{\kappa(A^T A)} - 1}{\sqrt{\kappa(A^T A)} + 1}\right)^m \|x_* - x_0\|_{A^T A}, \tag{1.3}$$

where x_0 is the initial guess, and $\kappa(A^T A) = \lambda_{\max}(A^T A)/\lambda_{\min}(A^T A)$.

From (1.3), it is obvious that a small $\kappa(A^T A)$, or close to one, will provide us a fine convergent boundary, vice versa. If A in (1.1) is ill-conditioned, the condition number of $A^T A$ will even be larger than the original one A, so that the convergence deteriorates consequently. We would like to utilize a preconditioner, which could make condition numbers better in the sense of convergence, to optimize the convergent boundary. For this reason, deflation and balancing preconditioners are suitable candidates. Now we define them as follow. Notice that A used below is not the system matrix of least squares problems (1.1) but just a general nonsigular matrix. Deflation preconditioners [6] are in these forms

$$P_{def} = I - AZE^{-1}Y^T, \tag{1.4}$$

for left precondition cases and

$$Q_{def} = I - ZE^{-1}Y^T A, \tag{1.5}$$

for right precondition ones, where $E = Y^T AZ$. Balancing preconditioners, proposed by Mandel [13], are illustrated below

$$P_{bal} = Q_{def} M^{-1} P_{def} + ZE^{-1}Y^T, \tag{1.6}$$

where $E = Y^T AZ$, Q_{def} and P_{def} are described in (1.4) and (1.5) respectively. And M is a nonsingular preconditioning matrix. Whereas the purpose of this paper focuses on the influence of deflation and balancing preconditioners related to least squares problems, we just set M as I, the identity matrix, for simplicity. Y and Z, here, are matrices of size $n \times r$, where $r \ll n$, and they also denote the deflation subspace which gives rise to the improved condition number. On the option of Y and Z, both of the two matrices should be full-ranked but we do not assume

that they are combined with eigenvectors for generality. Also we expect that Y and Z could make $E = Y^T AZ$ easy to compute, especially when inverting E. The balancing preconditioner has been analyzed by several authors in [8, 9, 10]. The details of such preconditioners will be stated in the following sections.

In this paper, what we concern about first is the reason why we choose GMRES instead of CGLS as the strategy for solving least squares problems. As we know, Krylov subspace methods can be divided into four different classes, and the typical Krylov subspace methods, such as CG, FOM [20], GMRES, BiCG and SYMMLQ [17], are all derived from the four approaches. On this preliminary, we propose that GMRES, to which mininum norm residual approach [22] leads, is a suitable method for least squares problems. In [10], Prof. Ken Hayami constructed a variant of the GMRES method for least squares problems. The ill-conditioned system matrices still exist and hamper convergence behaviors along iterative process in the situation that choosing an auxiliary matrix in Prof. Ken's methods without considering the improvement of condition numbers. Hence we precondition the variant of GMRES, named as BAGMRES in [10], with deflation and balancing preconditioners to optimize the spectral distribution so that the iterative Krylov subspace methods could achieve a better convergence rate.

Particulars of the option about iterative Krylov subspace methods will be stated in section 2. In section 3, the approach why and how the least squares problems could be solved by GMRES will be explained. The details of deflation and balancing preconditioners will be stated in section 4. KAGMRES with deflation and balancing preconditioners for least squares problems is presented in section 5. Then, numerical examples are demonstrated in section 6. Finally, conclusions are presented in section 7.

2. The option of Krylov subspace methods

For a large linear system

$$Ax = b, A \in R^{n\times n} \tag{2.1}$$

where A is nonsingular, we usually solve it through iterative Krylov subspace methods. We set x_0 as the initial guess, and then we get initial residual $r_0 = b - Ax_0$. The Krylov subspace is defined as follow

$$K_m(A, r_0) = span\{r_0, Ar_0, A^2r_0, ..., A^{m-1}r_0\}. \tag{2.2}$$

The approximate solution x_m, computed in the mth iteration, presents as a form belonged to the affine subspace $x_0 + K_m(A, r_0)$, i.e., $x_m \in x_0 + K_m(A, r_0)$. By this way, we limit approximate solutions in the affine subspace and expect to obtain more optimal approximate solutions. To get better approximate solutions, we should, at first, establish some regulations under which we search and compute the approximate solutions in the affine subspace $x_0 + K_m(A, r_0)$. As stated by Henk A. van der Vorst in the monograph [22], Krylov subspace methods can be distinguished into four different sorts:

(I). The Ritz-Galerkin approach. Under this approach we construct the x_m so that the residual, $r_m = b - Ax_m$, is orthogonal to the Krylov subspace, i.e., $b - Ax_m \perp K_m(A, r_0)$. In Krylov subspace methods, FOM and CG are both deduced based on this approach. The detailed process of deductions is demonstrated in the monograph [20]. However, the Ritz-Galerkin based methods may suffer from

expensive computation and storage caused by sophisticated recurrence relationship for approximate solutions.

(II). The Petrov-Galerkin approach. For overcoming the disadvantage of the Ritz-Galerkin approach, the Petrov-Galerkin is a regulation under which the residual, $r_m = b - Ax_m$, is orthogonal to other $k - dimensional$ subspace. For illustration, we could attain the biconjugate gradient method (BiCG) and the qusi-minimal residual method (QMR) if we select Krylov subspace $L_m(A^T, s_0)$ as the space to which the residual is orthogonal.

(III). The minimum norm error approach. In this approach the space where we look for the approximate solutions is different from the above ones. The approximate solutions, that is, based on the minimum norm error approach is constructed in $A^T K_m(A^T, r_0)$ and such that the 2-norm of error, $\|x_m - x\|_2$, is minimal. SYMMLQ method [17] and GMERR method [23] are designed along the minimum norm error approach.

(IV). The minimum norm residual approach. Similar to the minimum norm error approach, but in this approach we search for a approximate solution x_m in the space $K_m(A, r_0)$ and determine the optimality of x_m in the sense of minimal residual under 2-norm, *i.e.* $\min \|b - Ax_m\|_2$. GMRES, MINRES, and ORTHODIR are all derived from the the minimum norm residual approach. More information could be consulted in [20].

Along idea of the (IV), the approximate solution x_m, based on the minimum norm residual approach, satisfies that they make the 2-norm of residual minimal. This is coincident with the ultimate purpose that should be solved for the original least squares problems (1.1). And Krylov subspace methods based on (IV) can be all regarded as solvers of least squares problems, with a special case that $m = n$ in (1.1). On the other hand, we can not ensure that the approximate solutions based on (I), (II) and (III) are the optimal ones under the minimal norm of residual. For example, we assume that x_m^g and x_m^f are the approximate solutions computed by GMRES and FOM at mth step respectively. As we know, GMRES method is based on (IV) and FOM method on (I). To compare, from a abstractly angle, the effects of the two methods on solving least squares problems, we set the residual norms as $\|b - Ax_m^g\|_2$ for GMRES and $\|b - Ax_m^f\|_2$ for FOM. Then we have the following proposition.

Proposition 2.1. *We set* $\rho^g = \|b - Ax_m^g\|_2^g$ *and* $\rho^f = \min_{i=1,2,\ldots,m} \|b - Ax_i^f\|_2^f$. *Then we have the following relationship [20]:*

$$\rho^g \leq \rho^f. \tag{2.3}$$

Eq. (2.3) shows, obviously, that the approximate solution, within m-step iterations, through GMRES method are better than the one obtained by FOM for (1.1). Hence we select GMRES, a typical Krylov subspace method based on (IV), as the approach to solve least squares problems (1.1). Now GMRES method is shown as below.

Algorithm 1 GMRES with k restart [20].

1. select x_0 as the initial guess, $r_0 = b - Ax_0$ and $\nu_1 = r_0/\|r_0\|_2$
2. for $i = 1, 2, ..., m$
3. $\quad \omega_i = A\nu_i$
4. $\quad$ for $j = 1, 2, ..., i$
5. $\quad\quad h_{j,i} = (\omega_i, \nu_j)$
6. $\quad\quad \omega_i = \omega_i - h_{j,i}\nu_j$
7. $\quad$ endfor
8. $\quad h_{i+1,i} = \|\omega_i\|_2$
9. $\quad \nu_{i+1} = \omega_i/h_{i+1,i}$
10. $\quad$ Compute y_m to minimize $\|r_i\|_2 = \|\|r_0\|_2 e_1 - \overline{H}_i y\|_2$
11. $\quad$ if $\|r_i\|_2 < \tau$
12. $\quad\quad x_i = x_0 + [\nu_1, ..., \nu_i]y_i$
13. $\quad\quad$ stop
14. $\quad$ endif
15. endfor
16. set $x_0 = x_k$ and return to line 2 until convergence

The GMRES method, however, can not be applied to solve least squares problems directly. We have to translate the system matrix A in (1.1) into a square one by premultiplying a matrix, A^T in CGLS for instance. How to determine such a matrix denoted by K in order that the new system $KAx = Kb$ could be solved by GMRES is stated in the next section.

3. Auxiliary matrices for solving the least squares problems

Because the system matrix A in (1.1) is of size $m \times n$, where we just consider the situation $m > n$, the GMRES can not be utilized to obtain approximate solutions of (1.1). Hence, it is necessary to define an auxiliary matrix K of size $n \times m$ so that a new liear system $KAx = Kb$ satisfying GMRES solvers. We assume that K is certain an auxiliary matrix for the least squares problems (1.1), and the linear system handled by GMRES, therefore, turns to be $KAx = Kb$. Under the hypothesis, we structure a approximate solution under a Krylov subspace of the form

$$K_m(KA, \hat{r_0}) = span\{\hat{r_0}, KA\hat{r_0}, (KA)^2\hat{r_0}, ..., (KA)^{m-1}\hat{r_0}\}, \tag{3.1}$$

where $\hat{r_0} = Kr_0$. The approximate solution x_m, constructed in the Krylov subspace above through GMRES, is the optimal one to the new least squares problem as below

$$\min_x \|Kb - KAx\|_2. \tag{3.2}$$

For avoiding such problems like the one mentioned in Proposition 2.1, we should ensure that the approximate solution extracted from $min\|Kb - KAx\|_2$ is also the optimal approximation to the original question (1.1). Thanks to the work of Ken Hayami in [2,9,10,12], we could establish sufficient conditions to define a auxiliary matrix K by which a optimal approximation, to least squares problems (1.1), could be extracted from another least squares problems (3.2). In summary, the relative theorems to identify the auxiliary matrices are presented as below.

Theorem 3.1. *If and only if* $\mathrm{R}(A) = \mathrm{R}(K^TKA)$*, least squares problems* $\min \|b - Ax\|_2$ *and* $\min \|Kb - KAx\|_2$ *share the same optimal approximate solution* x_{opt} *for any* $b \in R^m$*.*

Proof. Following the assumption, it is obvious that $\|b - Ax_{opt}\|_2 = \min \|b - Ax\|_2$ and $\|Kb - KAx_{opt}\|_2 = \min \|Kb - KAx\|_2$. As mentioned in Chapter 5. and Chapter 6. in [20] , we have the relationships:

$$\|b - Ax_{opt}\|_2 \Leftrightarrow A^T(b - Ax_{opt}) = 0,$$

and also

$$\|Kb - KAx_{opt}\|_2 \Leftrightarrow (KA)^TK(b - Ax_{opt}) = 0 \Leftrightarrow A^TK^TK(b - Ax_{opt}) = 0.$$

Then, $\|b - Ax_{opt}\|_2 \Leftrightarrow \|Kb - KAx_{opt}\|_2$ if and only if $N(A^T) = N(A^TK^TK) \Leftrightarrow R(A) = R(K^TKA)$. □

Constructing auxiliary matrix K, however, through Theorem 3.1 is sophisticated and abstract, so we expect a more direct relationship between system matrix A and auxiliary matrix K to determine the latter. A theorem proposed by Ken Hayami in [10] is stated in the following.

Theorem 3.2. *The approximation solution of* $KAx = Kb$*, obtained through Krylov subspace iterative methods, minimizes* $\|b - Ax\|_2$ *if and only if* $\mathrm{R}(A) = \mathrm{R}(K^T)$*.*

Proof. See [10] for details. □

Furthermore, it is easy that $R(A) = R(AC^T)$ where C is nonsingular of size $n \times n$. If we construct K, depending on the relationship $R(A) = R(AC^T)$, as

$$K = CA^T, \tag{3.3}$$

the optimal approximate solution of (3.2) computed by GMRES is the optimal solution to least squares problems (1.1). Here we consider a nonsingular matrix C to construct auxiliary matrix K as (3.3), and then apply GMRES, illustrated in algorithm 1, to least squares problem (3.2), denoted by KAGMRES. We write it as below.

Algorithm 2 KAGMRES with k restart [10].

1. select x_0 as the initial guess, $\hat{r_0} = K(b - Ax_0)$ and $\nu_1 = r_0/\|r_0\|_2$
2. for $i = 1, 2, ..., m$
3. $\quad \omega_i = KA\nu_i$
4. $\quad$ for $j = 1, 2, ..., i$
5. $\quad\quad h_{j,i} = (\omega_i, \nu_j)$
6. $\quad\quad \omega_i = \omega_i - h_{j,i}\nu_j$
7. $\quad$ endfor
8. $\quad h_{i+1,i} = \|\omega_i\|_2$
9. $\quad \nu_{i+1} = \omega_i/h_{i+1,i}$
10. $\quad$ Compute y_m to minimize $\|\hat{r_i}\|_2 = \|\|\hat{r_0}\|_2 e_1 - \overline{H}_i y\|_2$
11. $\quad$ if $\|A^T r_i\|_2 < \tau$
12. $\quad\quad x_i = x_0 + [\nu_1, ..., \nu_i]y_i$
13. $\quad\quad$ stop
14. $\quad$ endif
15. endfor
16. set $x_0 = x_k$ and return to line 2 until convergence

The KAGMRES could be regarded as a special case of GMRES where the system matrix and right hand side are both premultiplied by CA^T. In summary, we look for the approximate solution of (3.2) in stead of solving (1.1) directly, and the solution of (3.2) is extracted from linear system $CA^TAx = CA^Tb$. We denote the linear system that is handled by KAGMRES directly as follow

$$\hat{A}x = \hat{b}. \tag{3.4}$$

Now we just need to determine a nonsingular matrix C of size $n \times n$ to construct the auxiliary matrix K, and then the approximate solution of (3.4) will give us the answer of (1.1). To analyze Algorithm 2 further, we expect the convergence bound of KAGMRES. At first, we give the convergence bound of GMRES for (3.4) as below.

Theorem 3.3. *$\hat{A} = X\Lambda X^{-1}$ is the spectral decomposition of the system matrix of (3.4), and $\Lambda = diag\{\lambda_1, \lambda_2, ..., \lambda_n\}$, $\lambda_n \geq \lambda_{n-1} \geq ... \geq \lambda_1 \geq 0$. Then it holds that*

$$\|\hat{r}_m\|_2 \leq 2\kappa_2(X)(1 - \frac{2}{\sqrt{\kappa(\hat{A})} + 1})^m \|\hat{r}_0\|_2, \tag{3.5}$$

where $\kappa_2(X) = \|X\|_2\|X^{-1}\|_2$ and $\kappa(\widehat{A}) = \frac{\lambda_n}{\lambda_1}$.

Proof. See [20] for instance. □

To identify X in Theorem 3.3, we consider the singular decomposition of $AC^{\frac{1}{2}}$ as $AC^{\frac{1}{2}} = U\Sigma V^T$. In this case,

$$\hat{A} = KA = CA^TA = C^{\frac{1}{2}}(AC^{\frac{1}{2}})^TAC^{\frac{1}{2}}C^{-\frac{1}{2}} = C^{\frac{1}{2}}V\Sigma^T\Sigma(C^{\frac{1}{2}}V)^T,$$

and where

$\Sigma = [D_\sigma, O]^T$, O is $0^{(m-n)\times n}$, $D_\sigma = diag\{\sigma_1, \sigma_2, ..., \sigma_n\}$, $\sigma_n \geq \sigma_{n-1} \geq, ..., \geq \sigma_1 \geq 0$

are the singular values of $AC^{\frac{1}{2}}$. Hence we have X easily that $X = C^{\frac{1}{2}}V$ and notice V is an unit matrix so that $\kappa_2(X) = \kappa_2(C^{\frac{1}{2}}V) = \sqrt{\kappa(C)}$. Now the convergence bound of KAGMRES writes as follow.

$$\|\hat{r}_m\|_2 \leq 2\sqrt{\kappa(C)}(1 - \frac{2}{\sqrt{\kappa(\hat{A})} + 1})^m\|\hat{r}_0\|_2. \tag{3.6}$$

We notice that the convergence bound of KAGMRES mainly depend on the condition number of $\hat{A}$, the smaller the better. However, if the system matrix A of (1.1) is ill-conditioned, that is to say the condition number of A is large, and C is choosed without considering the diminution of the condition number of KA, that is $\hat{A}$, the condition number of $\hat{A}$ will be equal to, or even larger than, the original one $\kappa(A)$. That hampers the convergence rate of KAGMRES, so a preconditioner aimed to improve the condition number is necessary in this situation. The deflation and balancing preconditioners are suitable choices for this purpose. These two preconditioners will be presented in the next section.

4. Deflation and balancing preconditioners

In this section, we will assume, for simplicity at first, that the deflation subspace is combined with the eigenvector columns in spectral analysis, although we just need to ensure the deflation subspaces, denoted by Y and Z, are full-ranked in practice. At the beginning, we will give a theorem to show the spectral distribution of a matrix A with the deflation preconditioner and balancing preconditioner in a special case that the deflation subspaces consist of the eigenvectors.

Theorem 4.1. *$Z = [z_1, z_2, ..., z_r]$ and $Y = [y_1, y_2, ..., y_r]$ satisfy that $\hat{A}z_i = \lambda_i z_i$ and $\hat{A}^T y_i = \lambda_i y_i$ respectively. The deflation preconditioner P_{def} and the balancing preconditioner P_{bal} are defined as (1.4) and (1.6) respectively. Then we have the following that*

$$\sigma(P_{def}\hat{A}) = \{0, ..., 0, \lambda_{r+1}, ..., \lambda_n\},$$

$$\sigma(P_{bal}\hat{A}) = \{1, ..., 1, \lambda_{r+1}, ..., \lambda_n\}.$$

Proof. $E = Y^T\hat{A}Z = diag(\lambda_1, \lambda_2, ..., \lambda_r)$ and $Y^TZ = I$. For $i = 1, 2, ..., r$,

$$P_{def}\hat{A}z_i = \hat{A}z_i - \hat{A}Z(diag(\lambda_1, \lambda_2, ..., \lambda_r))^{-1}Y^T\hat{A}z_i = 0.$$

For $i = r+1, r+2, ..., n$, $Y^Tz_i = 0$ and we give that

$$P_{def}\hat{A}z_i = \hat{A}z_i - \hat{A}Z(diag(\lambda_1, \lambda_2, ..., \lambda_r))^{-1}Y^T\hat{A}z_i = \lambda_i z_i.$$

The first conclusion $\sigma(P_{def}\hat{A}) = \{0, ..., 0, \lambda_{r+1}, ..., \lambda_n\}$ could be easily summarized. Similarly, for $i = 1, 2, ..., r$ expanding $P_{bal}\hat{A}z_i$ we have the following that

$$P_{bal}\hat{A}z_i = (I - ZE^{-1}Y^T)(I - \hat{A}ZE^{-1}Y^T)\hat{A}z_i + ZE^{-1}\hat{A}z_i = z_i$$

and, for $i = r+1, r+2, ..., n$,

$$P_{bal}\hat{A}z_i = \lambda_i z_i.$$

Hence, we have $\sigma(P_{bal}\hat{A}) = \{1, ..., 1, \lambda_{r+1}, ..., \lambda_n\}$. □

To compare the convergence bound with (3.5) in Theorem 3.3, we will give the convergence bound of the linear system

$$P_{def}\hat{A}x = P_{def}b. \tag{4.1}$$

It is obvious that the condition number of (4.1) is smaller than the one of (3.4), since the condition number of (4.1) is $\frac{\lambda_n}{\lambda_{r+1}}$, where $\frac{\lambda_n}{\lambda_1}$ of (3.4) and $\lambda_1 \leq \lambda_{r+1}$. Under this prerequisite, if the spectral decomposition of $P_{def}\hat{A}$ is of this form that $\hat{A} = X\Lambda_{def}X^{-1}$ where X is the eigenvectors of $\hat{A}$ and $\Lambda_{def} = diag(0, ..., 0, \lambda_{r+1}, ..., \lambda_n)$, we chould easily have the convergence bound of (4.1) as follow

$$\|P_{def}\hat{r}_m\|_2 \leq 2\kappa_2(X)(1 - \frac{2}{\sqrt{\kappa(P_{def}\hat{A})}})^m \|P_{def}\hat{r}_0\|_2. \tag{4.2}$$

It exists that$\hat{A}$ and $P_{def}\hat{A}$ share the same eigenvectors, this is $P_{def}\hat{A} = X\Lambda_{def}X^{-1}$. (See details in [4]) With $\kappa(P_{def}\hat{A}) < \kappa(\hat{A})$ as stated above, we could, therefore, have conclusion that the KAGMRES with deflation preconditioner, formed as (4.1) for example, have a faster convergence than (3.4).

Similarly we have the convergence bound of KAGMRES with balancing preconditioner as below

$$\|P_{bal}\hat{r}_m\|_2 \leq 2\kappa_2(X)(1 - \frac{2}{\sqrt{\kappa(P_{bal}\hat{A})}})^m \|P_{bal}\hat{r}_0\|_2. \tag{4.3}$$

That is to say the balancing preconditioner have a property to fast the convergence of GMRES resembling deflation. However we notice that the system matrix $\widehat{A}$ in (3.4) preconditioned by deflation may be singular. To guarantee KAGMRES convergence, it is necessary to obtain morn properties about P_{def} and P_{bal}. For $\frac{\lambda_n}{\lambda_1} \geq \frac{\lambda_n}{\lambda_{r+1}}$, the deflation preconditioner is better than the balancing precondition from the angle of improving condition numbers. And Yogi A. Erlangga and Reihard Nabben have proved it in [4]. Furthermore P_{bal} do not make $P_{bal}\hat{A}$ singular so that KAGMRES with balancing preconditioner will converge. We, hence, have the proposition next.

Proposition 4.1. *KAGMRES with deflation preconditioner will converge and is faster than KAGMRES with balancing preconditioner.*

We have discussed some properties of deflation and balancing preconditioners under an assumption that the deflation subspaces, Z and Y, is combined with the eigenvectors of $\hat{A}$. Under this precondition, it is manifest that these two preconditioners could improve the condition numbers effectively through changing the spectral distributions. Nevertheless we have to compute the eigenvalues and the corresponding eigenvectors at first. Even though we do not consider the round-off error in floating-point calculation, the expensive computation and storage for the eigenvalues and eigenvectors lead such an idea which is more in theory but not in

practice. For this reason the effection of the two preconditioners with arbitrary full-ranked matrix Z and Y as deflation subspace turns to importance. For generality, the spectral distributions of $P_{def}\widehat{A}$ and $P_{bal}\widehat{A}$ with arbitrary full-ranked matrix Z and Y will be presented in the following.

Theorem 4.2. *The deflation preconditioner and the balancing preconditioner are defined as (1.4) and (1.6) respectively. Z and Y are arbitrary full-ranked matrices of size $n \times r$ where $r \ll n$. Assume the spectrum of $P_{def}\widehat{A}$ is of this form*

$$\sigma(P_{def}\hat{A}) = \{0, ..., 0, \mu_{r+1}, ..., \mu_n\},$$

we have the spectrum of $P_{bal}\widehat{A}$ as

$$\sigma(P_{bal}\hat{A}) = \{1, ..., 1, \mu_{r+1}, ..., \mu_n\},$$

vice versa.

Proof. Z and Y are arbitrary full-ranked matrices. Expand $P_{def}\widehat{A}Z$ with $E = Y^T\widehat{A}Z$ and we have

$$P_{def}\hat{A}Z = \hat{A}Z - \hat{A}ZE^{-1}Y^T\hat{A}Z = 0.$$

Similarly we have

$$P_{bal}\hat{A}Z = Q_{def}P_{def}\hat{A}Z + ZE^{-1}Y^T\hat{A}Z = Z.$$

Here we obtain the first r eigenvalues of $P_{def}\hat{A}$ and $P_{bal}\hat{A}$. For $i = r+1, r+2, ..., n$, we set μ_i as eigenvalues of $P_{def}\hat{A}$ and $\tilde{z}_i$ as corresponding eigenvectors, that is $P_{def}\hat{A}\tilde{z}_i = \mu_i\tilde{z}_i$. We consider $Q_{def}\tilde{z}_i \neq 0$ and we have the relation next

$$\begin{aligned} P_{bal}\hat{A}Q_{def}\tilde{z}_i &= Q_{def}P_{def}\hat{A}Q_{def}\tilde{z}_i + ZE^{-1}Y^T\hat{A}Q_{def}\tilde{z}_i \\ &= Q_{def}P_{def}\hat{A}Q_{def}\tilde{z}_i = Q_{def}P_{def}\hat{A}\tilde{z}_i = \mu_i Q_{def}\tilde{z}_i. \end{aligned}$$

$P_{bal}A$ have eigenvectors as the form of $Q_{def}\tilde{z}_i$ corresponding to μ_i and we obtain the conclusion stated above.

Similarly we could conclude, on the condition

$$\sigma(P_{bal}\hat{A}) = \{1, ..., 1, \mu_{r+1}, ..., \mu_n\},$$

that

$$\sigma(P_{def}\hat{A}) = \{0, ..., 0, \mu_{r+1}, ..., \mu_n\}.$$

□

We realize, with Theorem 4.1 and Theorem 4.2, that no matter what full-ranked matrices we choose as the deflation subspace the spectral distributions are similar in form. To any linear system $Ax = b$, we take the condition number of system matrix A, abstractly, as the main criterion to judge convergence rate in Krylov iterative methods. And a small condition number is better than a large one in the sense of convergence. In a general case, we just select full-ranked matrices Y and Z, but not such matrices consisted of the eigenvectors of $\hat{A}$ and $\hat{A^T}$ respectively, as the deflation subspaces utilized in (1.4) and (1.6). The condition numbers, in this situation, of $P_{def}\hat{A}$ and $P_{bal}\hat{A}$ are expressed as $\kappa(P_{def}\hat{A}) = \frac{\mu_n}{\mu_{r+1}}$ and $\kappa(P_{bal}\hat{A}) = max\{\frac{\mu_n}{\mu_{r+1}}, \frac{\mu_n}{1}\}$ respectively.

Along with a feasible and theoretical angle of view, we give the following two assumptions.

Assumption 4.1 The system matrix $\hat{A}$ of (3.4) has real eigenvalues. The eigenvalues of the system matrix $\widehat{A}$, without preconditioning, are denoted as λ_i, where $\lambda_i < \lambda_j$ if and only if $i \leq j$. There is existing a j so that there is also existing i's satisfying $\lambda_i \leq 1$.

If all eigenvalues of the system matrix $\hat{A}$ are larger than one, the balancing preconditioner is insignificance. Also, the effection of the deflation preconditioner is hampered in some sense.

Assumption 4.2 The dimension of deflation subspace r is large enough to guarantee μ_{r+1}, the $(r+1)$-th eigenvalue of the preconditioned system matrix $P_{def}\widehat{A}$ or $P_{def}\widehat{A}$, is larger than or equal to one.

Under this assumption, the deflation and the balancing preconditioners both effectively discard the smallest eigenvalues, which may course a bad condition number, from spectrum.

With the above two assumptions, naturally we could obtain the theorem next.

Theorem 4.3. *$\kappa(\hat{A})$, $\kappa(P_{def}\hat{A})$ and $\kappa(P_{bal}\hat{A})$ are condition numbers of the system matrix in (3.4), preconditioned system matrices $\kappa(P_{def}\hat{A})$ and $\kappa(P_{bal}\hat{A})$ respectively. Then they hold the relationship as below,*

$$\kappa(\hat{A}) \geq \kappa(P_{bal}\hat{A}) \geq \kappa(P_{def}\hat{A}).$$

Proof. We set the eigenvalues, except zero and one, of P_{def} and P_{bal} as μ_i and the eigenvalues of $\hat{A}$ as λ_i. Under assumption 4.4 and assumption 4.5, we have $\mu_{r+1} \geq 1 \geq \lambda_1$, and then $\kappa(P_{bal}\hat{A}) = \frac{\mu_n}{1} \geq \frac{\mu_n}{\mu_{r+1}} = \kappa(P_{def}\hat{A})$. Obvious is $\mu_i \leq \lambda_i$. (details in [11]) Hence, it holds that $\kappa(\hat{A}) = \frac{\lambda_n}{\lambda_1} \geq \frac{\mu_n}{1} = \kappa(P_{bal}\hat{A})$. In summary, we could conclude that $\kappa(\hat{A}) \geq \kappa(P_{bal}\hat{A}) \geq \kappa(P_{def}\hat{A})$. □

In conclusion, utilizing any full-ranked matrices with an appropriate dimension as deflation subspace, the deflation and the balancing preconditioners could both improve the solving system through optimizing condition numbers. For a least squares problem with an ill-conditioned system matrix, if the auxiliary matrix K is constructed without consideration of optimizing condition number, it is necessary to use the deflation preconditioner or the balancing preconditioner for improving the spectral distribution of $\hat{A}$ in order to accelerate Krylov subspace methods, KAGMRES as example. In the following section, details in implementation of preconditioned Krylov subspace methods for least squares problems will be presented.

5. Preconditioned Krylov subspace methods for least squares problems

Through the past sections, we found that we select an auxiliary matrix K to translate the least squares problem (1.1) into (3.2) and solve (3.2) by applying KAGMRES to (3.4). When the system matrix A of original linear system is ill-conditioned

and the auxiliary matrix K can not make the condition number of KA, or $\hat{A}$, smaller, we utilize the deflation or the balancing preconditioners to accelerate the iterative Krylov subspace methods, KAGMRES in this paper. Hence, we have to focus on the following two questions that (i) determination of deflation subspace Z and Y, and (ii) the process of computation for solving the least squares problem (1.1).

5.1. Choice of deflation subspace Z and Y

Choosing z_i and y_i as columns of Z and Y respectively, where $\hat{A}z_i = \lambda_i z_i$ and $\hat{A}^T y_i = \lambda_i y_i$, is a appropriate option in theory, but the approach is hard to achieve. For generality, we just need to construct a matrix of full rank. In this paper, we construct the deflation subspace Y and Z based on domain decomposition, which has been proposed by Mansfield in [14] and cited by Nicolaides in [15].

We describe the construction of Z and Y along with Frank's work in [6]. The domain Ω is decomposed into k subdomains Ω_j, $j = 1, 2, ..., k$. Meanwhile we set up an index set θ_j and define it as $\theta_j = \{i | u_i \in \Omega_j\}$. There exists a one-to-one correspondence relationship between the index set θ_j and the subdomain Ω_j. And we just consider Ω_j's are connected, but nonoverlapping, subdomains covering Ω for simplicity. Therefore, we define elements of Z next,

$$z_{ij} = \begin{cases} 1, & i \in \theta_j, \\ 0, & i \notin \theta_j. \end{cases}$$

And we assume that another deflation subspace Y is equal to Z, with the feasibility proved by Franck and Vuik in [6]. Next we will give the algorithm to obtain Z.

Algorithm 3 Deflation subspace computation

1. Assume the dimension of $\hat{A}$ is n, and the deflation subspace Z is of size $n \times r$.
2. $\alpha = n/r$
3. if $\alpha \neq 0$
4. end
5. for $i = 1, 2, ..., n$; $j = 1, 2, ..., r$
6. $\quad z_{ij} = 0$
7. end
8. for $j = 1, 2, ..., r$
9. $\quad$ for $k = 1, 2, ..., \alpha$
10. $\quad i = k + \alpha(j - 1)$
11. $\quad z_{ij} = 1$
12. $\quad$ endfor
13. endfor

5.2. Computation process

Recall that we avoid solving least squares problems (1.1) directly, but make it into (3.4) and handle it with preconditioned KAGMRES. Notice that the process of applying GMRES, with deflation preconditioners, to (3.4) performs in three steps one by one. At first, we rewrite x as

$$x = (I - Q_{def})x + Q_{def}x.$$

And then we could easily get that $(I - Q_{def})x = ZE^{-1}Y^T\hat{A}x = ZE^{-1}Y^T\hat{b}$. Finally we apply GMRES to linear system $P_{def}\hat{A}u = P_{def}\hat{b}$ to extract approximation solution $\tilde{u}$. $Q_{def}x$ can be presented as $Q_{def}\tilde{u}$. Hence, with the deflation preconditioner the ultimate solution of (1.1) is in this form that

$$x = ZE^{-1}Y^T\hat{b} + Q_{def}\tilde{u}.$$

Choosing P_{bal} to precondition (3.4), we consider P_{bal} as a left-preconditioner and solve (3.4) by Left-Preconditioned KAGMRES [20]. The approximate solution extracted from Left-Preconditioned KAGMRES is the ultimate solution to (1.1).

On the option of the auxiliary matrix, we set C based on diagonal scaling by the utilization of the diagonal elements of A^TA for simplicity. That is $C = [diag(A^TA)]^{-1}$, and then we have the auxiliary matrix $K = CA^T$.

6. Numerical experiment

In this section, the numerical experiments will be presented to illustrate the effection of the deflation and balancing preconditioners when we select an iterative Krylov method for solving least squares problems. The CGLS method, regarded as a typical method for least squares problems, will be used as compare item. The main function of deflation and balancing preconditioners are effective improvement on the condition number for accelerating convergence rate. Hence, it is not necessary to impose the preconditioners on a well-conditioned system matrix. In this numerical experiment, we only select such least squares problems which have ill-conditioned system matrix as examples. The system matrices are constructed by the MATLAB routine "sprandn(m, n, density, rc)", where sprandn(m, n, density, rc) is a random, m-by-n, sparse matrix with approximately $density \times m \times n$ normally distributed nonzero entries. The last term "rc" presents the reciprocal of condition number approximately, that is to say the smaller is "rc" the more ill-conditioned is the system matrix of (1.1). The right-hand side vector b is generated by MATLAB routine "randn(m, 1)". Considering the special form of the preconditioned Krylov subspace [4], in which we search for approximate solutions, the initial guesses are presented

$$x_0^{def} = (0, 0, ..., 0)^T$$

and

$$x_0^{bal} = ZE^{-1}Y^T\hat{b}$$

for deflation and balancing preconditioned KAGMRES respectively. The following numerical experiments are performed with the dimension of deflation subspace $r = 50$ and precision $\tau = 1.1 \times 10^{16}$.

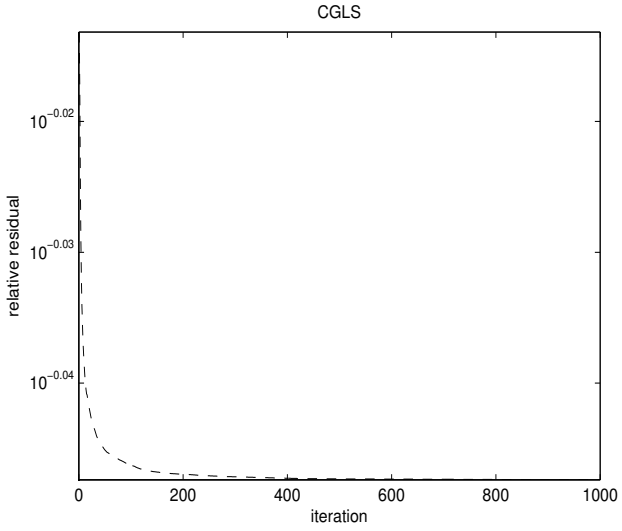

Figure 1. $\|A^T r\|_2/\|A^T b\|_2$ *vs.* iterations ($m = 5000$, $n = 1000$, density=0.01, condition number=10^6, $r = 50$)

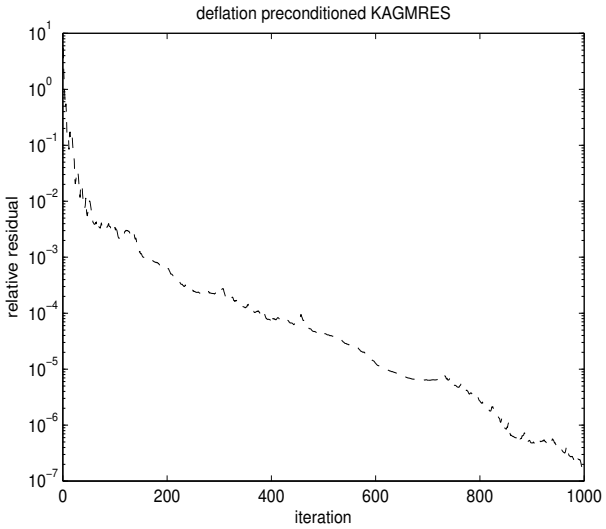

Figure 2. $\|A^T r\|_2/\|A^T b\|_2$ *vs.* iterations ($m = 5000$, $n = 1000$, density=0.01, condition number=10^6, $r = 50$)

With an ill-conditioned system matrix marked by condition number=10^6, Fig. 1, Fig. 2 and Fig. 3 indicate that convergence rate of preconditioner KAGMRES is much better than the one of CGLS, and effections of deflation and balancing preconditioners are similar in the way of convergence.

The same conclusion could still be illustrated by Fig. 4, Fig. 5 and Fig. 6, where the system matrix is more ill-conditioned for setting condition number=10^8.

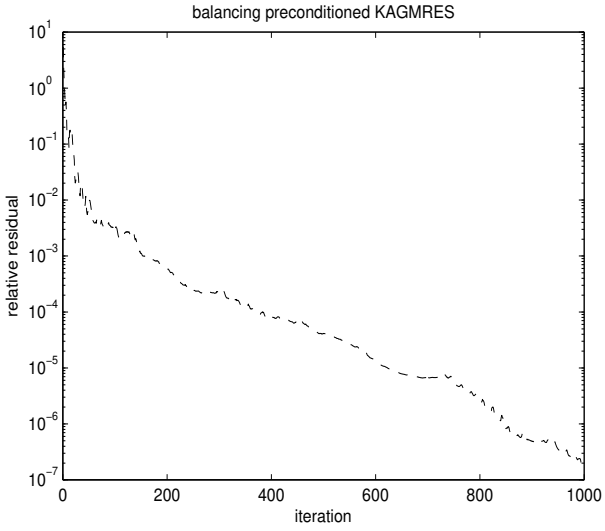

Figure 3. $\|A^T r\|_2/\|A^T b\|_2$ *vs.* iterations ($m = 5000$, $n = 1000$, density=0.01, condition number=10^6, $r = 50$)

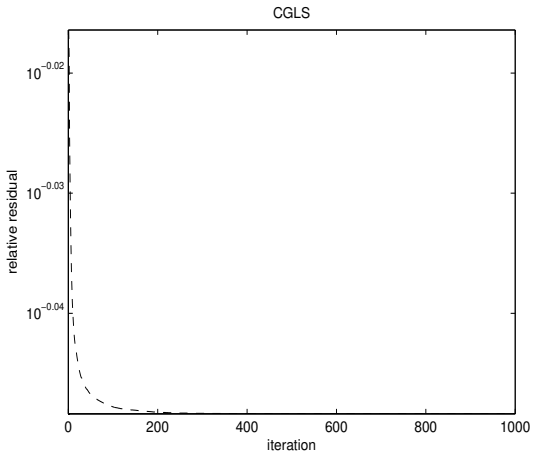

Figure 4. $\|A^T r\|_2/\|A^T b\|_2$ *vs.* iterations ($m = 5000$, $n = 1000$, density=0.01, condition number=10^8, $r = 50$)

The above six numerical experiments state the fact that the deflation and balancing preconditioners improve the convergence rate of iterative Krylov subspace method, KAGMRES as example, effectively through optimizing condition number.

7. Conclusions

For least squares problems, we choose GMRES, which is derived from the minimum norm residual approach, as the main strategy because of the relationship between

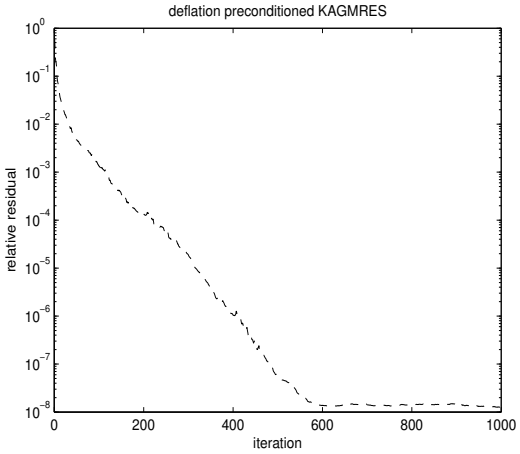

Figure 5. $\|A^T r\|_2/\|A^T b\|_2$ *vs.* iterations ($m = 5000$, $n = 1000$, density=0.01, condition number=10^8, $r = 50$)

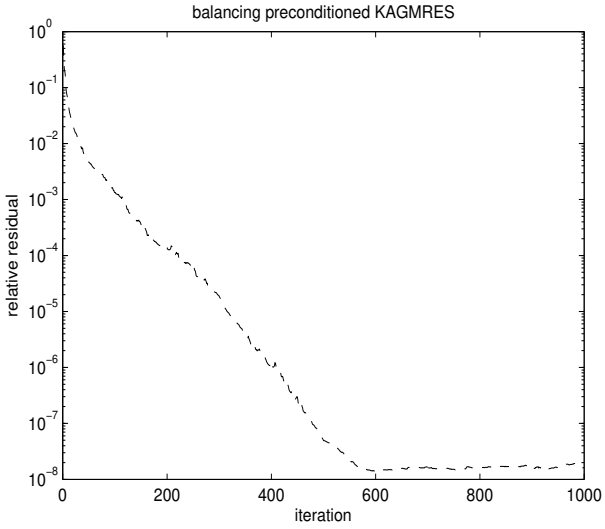

Figure 6. $\|A^T r\|_2/\|A^T b\|_2$ *vs.* iterations ($m = 5000$, $n = 1000$, density=0.01, condition number=10^8, $r = 50$)

such approach and the least squares problems. (See Proposition 2.1 for instance) In order to utilize GMRES to solve the least squares problem $min\|b-Ax\|_2$, we establish the principle that constructing auxiliary matrix K with a nonsingular matrix C as the form $K = CA^T$. Now, the least squares problem $min\|b-Ax\|_2$ is translated into $min\|Kb-KAx\|_2$. We, then, have the Algorithm 2 KAGMRES, which handle a new linear system as $\hat{A}x = \hat{b}$ directly to extract the optimal approximate solution to $min\|Kb - KAx\|_2$. To overcome the problems brought an ill-conditioned system matrix A, we precondition the linear system $\hat{A}x = \hat{b}$ by the deflation and

the balancing preconditioners so that achieving a better convergence. Comparing with CGLS, Krylov subspace methods with deflation and balancing preconditioners are effective ways for the solving least squares problems, even though the system matrix is ill-conditioned.

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