ISSN 1749-3889 (print), 1749-3897 (online)
International Journal of Nonlinear Science
Vol.17(2014) No.2,pp.188-192

Modified Block Jacobi-Davidson Method for Solving Large Sparse Eigenproblems

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(Received 20 June 2013 , accepted 11 March 2014)

Abstract: The Jacobi-Davidson Method is an efficient eigenvalue solver which uses an inner-outer scheme. In the outer iteration one tries to approximate an eigenpair while in the inner iteration a linear system has to be solved, often iteratively. The more time-consuming computation lies in solving the linear system which is called correction equations. To handle the inexact solution of the correction equations, we use extrapolation technique to solve the correction equations. Furthermore, we use a a class of preconditioners when solving the correction equations with Krylov subspace methods, such as GMRES(m). Numerical experiments show that the new algorithm is efficient.

Keywords: Jacobi-Davidson algorithm; correction equation; extrapolation technique;preconditioner

1 Introduction

In many fields of science and engineering technology, we often need to calculate several extreme (maximum or minimum) or internal eigenvalues and corresponding eigenvectors of large sparse symmetric matrix. In 2000, Sleijpen and Van der Vorst [6] combined correction method of Jacobi with inner -outer iterative method of Davidson [4, 5] and proposed Jacobi-Davidson method. This method has good stability and can achieve a fast convergence speed of non-diagonally dominant or non-normal matrices. At present, the Jacobi-Davidson method is one of the most effective methods for solving eigenvalue problems. But when the matrix has multiple eigenvalues , the validity and reliability of Jacobi-Davidson method will decrease. To overcome this, block Jacobi-Davidson method was proposed and it can calculate the multiple eigenvalues of matrix.

Algorithm 1(Block Jacobi-Davidson Method)

1 input: matrix A, the maximum dimension of projection subspace m*, block size* l*, column orthonormal matrix* V_1 *with size* $n \times l$*;*

2 For $k = 1, 2, \cdots, m$.

(1) compute $V_k^T AV_k$*;*

(2) compute l *eigenpairs* $(\lambda_i^{(k)}, y_i^{(k)})$*,* $(i = 1, 2, \cdots, l)$ *of* H_k.

(3) compute Ritz vector $(\phi_i^{(k)}, y_i^{(k)})$*,* $(i = 1, 2, \cdots, l)$*;*

(4) compute residual vector $r_i^{(k)} = (A - \lambda_i^{(k)} I)\phi_i^{(k)}$*,* $(i = 1, 2, \cdots, l)$.

Test for convergence. Stop if $\|r_i^{(k)}\| < Tol$ *is satisfied.*

(5) Solve

$$\begin{cases} (I - \phi^{(k)}\phi^{(k)^T})(A - \lambda_i^{(k)} I)((I - \phi^{(k)}\phi^{(k)^T}))t_i^{(k)} &= -r_i^{(k)} \\ \phi^{(k)^T} t_i^{(k)} &= 0, \end{cases} \quad (i = 1, 2, \cdots, l).$$

Get new matrix $T_k = [t_1^{(k)}, \cdots, t_l^{(k)}]$*, where* $\phi^{(k)} = (\phi_1^{(k)}, \cdots, \phi_i(k))$.

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IJNS.2014.04.15/803

(6) $V_{k+1} = MGS(V_k, T_k)(ModifiedGram - Schmidt)$.

The block Jacobi Davidson algorithm is divided into two layers of inner and outer iteration, the outer iteration calculates eigenpairs of matrix and the inner iteration solves the linear system which is called correction equations. The main cost lies in the inner iterations. In the Jacobi-Davidson method, each iteration step requires the solution of the correction equation

$$\begin{cases} (I-\phi^{(k)}{\phi^{(k)}}^T)(A-\lambda_i^{(k)}I)((I-\phi^{(k)}{\phi^{(k)}}^T))t_i^{(k)} &= -r_i^{(k)} \\ {\phi^{(k)}}^T t_i^{(k)} &= 0, \end{cases} \quad (i=1,2,\cdots,l), \tag{1}$$

where $\phi^T\phi = I$. In this work, we propose a modified version of the block Jacobi Davidson algorithm by introduce a extrapolation parameter, which can get eigenvalues more efficiently.

The paper is organized as follows. In section 2, the Modified Block Jacobi-Davidson Method will be given,and the optimal parameter of ω is discussed.Then a preconditioning technique is used in GMRES(m) algorithm when solving the correction equation. While in section 3, numerical results are presented to illustrate the behavior of the new algorithms.

2 Modified Block Jacobi-Davidson Method

With the approaching degree enhancement, the condition number of the coefficient matrix equations will go bad, we can use the extrapolation technique to overcome this.

If the solution of (1) reads as,

$$t^{(k)} = Gt^{(k-1)} + C. \tag{2}$$

Let

$$t^{(k)} = \omega(Gt^{(k-1)} + C) + (1-\omega)t^{(k-1)} = [\omega G + (1-\omega)I]t^{(k-1)} + \omega C, \tag{3}$$

where $\omega \neq 0$ is a parameter.

Then we get a new iterative method. Apparently, when $\omega = 1$ the iteration formula (3) is the original (2).

This extrapolate method converges if and only if $\rho(G_\omega) < 1$. If we only know all the eigenvalues of G contained in the interval $[a,b]$, then the eigenvalues of $G_\omega = \omega G + (1-\omega)I$ are located in the interval with the endpoints of $\omega a + 1 - \omega$ and $\omega b + 1 - \omega$.

Let $\lambda(A)$ denote the set of eigenvalues of matrix A, Then

$$\rho(G_\omega) = \max_{\lambda\in\lambda(G_\omega)} |\lambda| = \max_{\lambda\in\lambda(G_\omega)} |\omega\lambda + 1 - \omega| \leq \max_{a\leq\lambda\leq b} |\omega\lambda + 1 - \omega|.$$

When $1 \notin [a,b]$, we can choose ω such that $\rho(G_\omega) < 1$

Theorem 1 *If all the eigenvalues of G are real and locate in the interval* $[a,b]$*, and* $1 \notin [a,b]$*, then the optimal parameter of* ω *is* $\omega_{opt} = \frac{2}{2-a-b}$*. And* $\rho(G_{\omega_{opt}}) \leq 1 - |\omega_{opt}|d$*, where* d *is the distance from* 1 *to* $[a,b]$.

Proof. Function $\max_{a\leq\lambda\leq b} |\omega\lambda+1-\omega|$ has a minimum value when $|\omega a+1-\omega| = |\omega b+1-\omega|$, which results in $\omega_{opt} = \frac{2}{2-a-b}$.

Since $1 \notin [a,b]$, so either $a > 1$ or $b < 1$.

For $a \leq b < 1$, we have $\omega_{opt} > 0$ and $d = 1 - b$.

All the eigenvalues of $G_{\omega_{opt}}$ satisfies the inequality

$$\omega_{opt}a + 1 - \omega_{opt} \leq \lambda \leq \omega_{opt}b + 1 - \omega_{opt},$$

so we have $\lambda \leq \omega_{opt}b + 1 - \omega_{opt} = 1 + \omega_{opt}(b-1) = 1 - \omega_{opt}d$, and $\lambda \geq \omega_{opt}a + 1 - \omega_{opt} = -1 + \omega_{opt}d$. As a result, we get $-1 + \omega_{opt}d \leq \rho(G_{\omega_{opt}}) \leq 1 - \omega_{opt}d$.

Similarly, for $1 < a \leq b$, we can obtain the same results. The proof is completed. ■

We often use Krylov subspace methods to solve the correction equation (1). Restarted GMRES method is well known and widely used which is listed below.

Algorithm 2 (GMRES(m))

1 Compute $r_0 = b - Ax_0$, $\beta = \|r_0\|_2$ and $v_1 = \frac{r_0}{\beta}$

2 Generate the Arnoldi basis and the matrix $\overline{H}_m$ by using the Arnoldi algorithm starting with v_1

3 Compute y_m which minimizes $\|\beta e_1 - \overline{H}_m y\|_2$ and $x_m = x_0 + V_m y_m$

4 If satisfied then stop, else set $x_0 := x_m$ and Go To 1

We can use preconditioning technique when solving the correction equation with GMRES(m). The aim of preconditioning is to accelerate the convergence speed by making the eigenvalues of matrix A located in the complex plane as cluster as possible.

There are many techniques to construct preconditioners, such as incomplete LU decomposition, incomplete Cholesky decomposition and so on. Incomplete LU decomposition method is discussed here. The matrix A is divided into four blocks and the corresponding LU decomposition is given as follows.

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ & U_{22} \end{pmatrix} \tag{4}$$

where A_{11} is a matrix with size $d_1 \times d_1$,A_{22} is a matrix with size $(n-d_1) \times (n-d_1)$. From (4),we have

$$A_{11} = L_{11}U_{11} \tag{5}$$
$$A_{12} = L_{11}U_{12} \tag{6}$$
$$A_{21} = L_{21}U_{11} \tag{7}$$
$$A_{22} = L_{21}U_{12}+L_{22}U_{22} \tag{8}$$

Algorithm 3 Block ILU algorithm

1 For an Incomplete LU decomposition of the block matrix A_{11}, get L_{11}, U_{11}

2 Compute B_1, the inverse matrix of L_{11}, which is still an unit lower triangular matrix

3 $U_{12} = L_{11}^{-1}A_{12} = B_1A_{12}$

4 Compute C_1, the inverse matrix of U_{11}, which is still an upper triangular matrix

5 $L_{21} = A_{21}U_{11}^{-1} = A_{21}C_1$

6 denote $A'_{22} = A_{22} - L_{21}U_{12}$, the LU decomposition $A'_{22} = L_{22}U_{22}$

The LU decomposition of A'_{22} can always be done by block calculation, as long as a proper size of the block is selected. Furthermore calculation of the inverse matrix in the algorithm makes full use of the characteristics of triangular matrix to eliminate unnecessary computation, and thus the calculation speed is improved.

3 Numerical Experiment

In this section, numerical experiments are implemented by Matlab 6.5 . The initial matrix is generated randomly and its column vectors are orthonormal. To be convenient, the block Jacobi-Davidson method is denoted as BJD and modified Jacobi-Davidson method is denoted as MBJD.The block Jacobi-Davidson method with ILU decomposition preconditioner when solving correcting equation is denoted as ILUBJD.

Example 1 *Consider matrix A which is of order 1600×1600, where the matrix B is of order 40×40.*

$$A = \begin{pmatrix} B & -I & & & & \\ -I & B & -I & & & \\ & \cdots & \cdots & \cdots & & \\ & & \cdots & \cdots & \cdots & \\ & & & \cdots & \cdots & -I \\ & & & & -I & B \end{pmatrix},$$

where

$$B = \begin{pmatrix} 4 & -1 & & & & \\ -1 & 4 & -1 & & & \\ & \cdots & \cdots & \cdots & & \\ & & \cdots & \cdots & \cdots & \\ & & & \cdots & \cdots & -1 \\ & & & & -1 & 4 \end{pmatrix}.$$

The computed three biggest eigenvalues together with CPU times by (Modified) block Jacobi-Davidson Method are listed in the Table 1. The Tolerances for the two methods are 10^{-5}. The results show that the modified block Jacobi-Davidson method can accelerate the convergence speed by using extrapolation technique.

Table 1: The results for the biggest three eigenvalues of A

Algorithm	eigenvalues	CPU time (s)
	7.9883	
BJD	7.9707	184.15
	7.9707	
	7.9883	
MBJD	7.9707	166.23
	7.9707	

Example 2 *Consider matrix A which is of order 500×500, where the matrix B is of order 20×20.*

$$A = \begin{pmatrix} B & -I & & \\ -I & B & \cdots & \\ & \cdots & \cdots & -I \\ & & -I & B \end{pmatrix},$$

where

$$B = \begin{pmatrix} 4 & -0.4 & & \\ -0.4 & 4 & \cdots & \\ & \cdots & \cdots & -0.4 \\ & & -0.4 & 4 \end{pmatrix}.$$

Table 2: The results for the biggest four eigenvalues of A

Algorithm	eigenvalues	CPU time (s)
	6.7756	
BJD	6.7754	16.32
	6.7321	
	6.7315	
	6.7756	
ILUBJD	6.7754	15.19
	6.7321	
	6.7315	

The computed four biggest eigenvalues together with CPU times by block Jacobi-Davidson Method with ILU preconditioner are listed in the Table 2. The Tolerances for the two methods are 10^{-5}. The results show that the block Jacobi-Davidson method with ILU decomposition preconditioner when solving the correction equation can accelerate the convergence speed .

Acknowledgments

The authors would like to thank the referees for their valuable comments and suggestions which improve the manuscript greatly.

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