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PRECONDITIONING BLOCK LANCZOS ALGORITHM FOR SOLVING SYMMETRIC EIGENVALUE PROBLEMS [*1)]

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Abstract

A preconditioned iterative method for computing a few eigenpairs of large sparse symmetric matrices is presented in this paper. The proposed method which combines the preconditioning techniques with the efficiency of block Lanczos algorithm is suitable for determination of the extreme eigenvalues as well as their multiplicities. The global convergence and the asymptotically quadratic convergence of the new method are also demonstrated.

Key words: eigenvalue, eigenvector, sparse matrices, Lanczos method, preconditioning

1. Introduction

The Lanczos process is an effective method [1, 2, 14, 21] for computing a few eigenvalues and corresponding eigenvectors of a large sparse symmetric matrix $A \in \mathbf{R}^{n\times n}$. If it is practical to factor the matrix $A-\rho I$ for one or more values of ρ near the desired eigenvalues, the Lanczos method can be used with the inverted operator and convergence will be very rapid[5,10,22]. In practical applications, however, the matrix A is usually large and sparse, so factoring A is either impossible or undesirable. The Lanczos algorithm can suffer from convergence problem if the desired eigenvalues are not well separated from the rest of the spectrum.

The conjugate gradient method [11] for solving linear equations has also convergence problem if the distribution of eigenvalues is unfavorable. Convergence of the conjugate gradient method can be improved by preconditioning techniques [3, 15, 16]. It would also be desirable to improve the convergence of the Lanczos algorithm with preconditioning techniques, but this is not straightforward. Preconditioning can be applied indirectly to eigenvalue problems by using the preconditioned conjugate gradient method or the preconditioned SOR method to solve equations for inverse iteration [6, 7, 20], the Rayleigh quotient iteration [23, 24] and shift-and-invert Lanczos method [5, 10, 22].

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The generalized Davidson method [17, 18] gives a more direct preconditioning approach to eigenvalue problems. The method generates a subspace with the operator $N(\rho) = (M - \rho I)^{-1}(A - \rho I)$, where ρ is the most recent approximation to the desired eigenvalue, M is any approximation to A. $M - \rho I$ can be viewed as a preconditioner to $A - \rho I$. Morgan and Scott[19] transformed $N(\rho)$ to a symmetric operator $L^{-1}(A - \rho I)L^{-T}$ so that the Lanczos algorithm can be applied, where LL^T is the Cholesky factorization of the preconditioner $M - \rho I$. Certainly, the preconditioner $M - \rho I$ is required to be symmetric positive definite. Then they gave a preconditioning Lanczos algorithm (called the PL algorithm). However it is difficult to determine the multiplicity of the computed eigenvalues by using the PL algorithm and there are some errors in the PL algorithm and the proof of its convergence.

The method we will describe, the preconditioning block Lanczos algorithm (called the PBL algorithm), is an extension of the PL algorithm. A double iteration scheme is also used. The Rayleigh-Ritz procedure and a certain preconditioned matrix are used in the outside loop; the block Lanczos algorithm[4,9] is applied in the inside loop. The PBL algorithm not only enables us to detect the multiplicity of the computed eigenvalues, but affords us improved rates of convergence. This algorithm can be very efficient if the matrix is fairly sparse and an approximation inverse is easily available.

In section 2 we formulate the PBL algorithm and discuss the various steps of the computations. In section 3 we analyze the global convergence of the algorithm and asymptotically quadratic convergence with respect to the outer loop. Section 4 looks at some implementation details and gives numerical experiments where a comparison with the block Lanczos algorithm is investigated.

2. Preconditioning Block Lanczos (PBL) Algorithm

Let the eigenvalues $\lambda_i (i = 1, 2, \cdots, n)$ of the symmetric matrix A be ordered as follows

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_j \le \lambda_{j+1} \le \cdots \le \lambda_n \tag{1}$$

Suppose that we are interested in computing the j-th smallest eigenvalue and corresponding eigenvector of the matrix A. The preconditioning block Lanczos algorithm can be described as follows.

PBL Algorithm. Choose $m (m \ge j)$ linear independent vectors $x_i^{(0)} (i = 1, 2, \cdots, m)$, and let $X^{(0)} = [x_1^{(0)}, \cdots, x_m^{(0)}]$.

For $k = 0, 1, \cdots$, do 1) to 5)

1) Compute $A_k = X^{(k)^T} A X^{(k)}$, $B_k = X^{(k)^T} X^{(k)}$, and find the j smallest eigenvalues $\mu_1^{(k)}, \cdots, \mu_j^{(k)} (\mu_1^{(k)} \le \cdots \le \mu_j^{(k)})$ and corresponding eigenvectors $q_1^{(k)}, \cdots, q_j^{(k)}$ of the symmetric generalized eigenvalue problem

$$A_k q = \mu B_k q \tag{2}$$

and let $Q^{(k)} = [q_1^{(k)}, \cdots, q_j^{(k)}]$.

2) Choose M_k to be a symmetric positive definite matrix approximating $A - \mu_j^{(k)} I$, and compute the Cholesky factorization $M_k = L_k L_k^T$.

3) Define the matrix

$$W_k = L_k^{-1}(A - \mu_j^{(k)} I) L_k^{-T} \tag{3}$$

4) Run the block Lanczos algorithm with W_k and starting matrix $L_k^T X^{(k)} Q^{(k)}$ until the m smallest Ritz values $\theta_1^{(k)}, \cdots, \theta_m^{(k)}$ of W_k converge, and let $Y_1^{(k)} = [y_1^{(k)}, \cdots, y_m^{(k)}]$, where $y_i^{(k)} (i = 1, \cdots, m)$ is the Ritz vector associated with the Ritz value $\theta_i^{(k)}$.

5) Let

$$X^{(k+1)} = L_k^{-T} Y_1^{(k)} \tag{4}$$

Remark 2.1. In the case of $j = 1$ the PBL algorithm is an improvement of the PL algorithm[19]. There is an error in Step 5 of the PL algorithm (see [19] for symbols). In fact, $y_k^T W_k y_k$ generally is not equal to θ_k because (θ_k, y_k) is not an eigenpair of W_k and is only a Ritzpair which satisfied $-\theta_k \geq \|W_k y_k - \theta_k y_k\|$. So $x_{k+1}^T A x_{k+1} / x_{k+1}^T x_{k+1}$ does not equate to $\rho_k + \theta_k / x_{k+1}^T x_{k+1}$. The same mistake occurs in the proof of Theorem 1[19].

Remark 2.2. The generalized eigenvalue problem (2) is the Rayleigh-Ritz procedure of the matrix A with respect to the linear independent basis $X^{(k)}$ of the subspace $span(X^{(k)})$. We can use generalized Jacobi method or other methods available for solving the lower order (in general $m \ll n$) generalized eigenvalue problem[1,21].

Remark 2.3. The main cost of the PBL algorithm is in the block Lanczos loop. So it is important for the block Lanczos iteration to converge quickly. Convergence of the block Lanczos algorithm is strongly dependent on the eigenvalue distribution of W_k, or equivalently of $M_k^{-1}(A - \mu_j^{(k)} I)$. Here the preconditioning improves the distribution of eigenvalues just as it does for the generalized Davidson method.

3. Convergence of the PBL Algorithm

We now analyze the convergence of the PBL algorithm. The preconditioner does not need to be an accurate approximation. If there is boundedness, then the sequence $\{\mu_j^{(k)}\}$ in the PBL algorithm converge to the j-th smallest eigenvalue of A at an asymptotically quadratic rate.

Let us first introduce a lemma.

Lemma[12]**.** *Let A and B be symmetric and positive definite matrices of order n, respectively, and $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ denote the eigenvalues of the generalized eigenvalue problem $Ax = \lambda Bx$. Suppose that X is an $n \times m (m \leq n)$ matrix with $rank(X) = m$, $\widehat{A} = X^T A X, \widehat{B} = X^T B X$. If $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_m$ are the eigenvalues of the generalized eigenvalue problem $\widehat{A} q = \mu \widehat{B} q$, then*

$$\lambda_i \leq \mu_i, i = 1, 2, \cdots, m \tag{5}$$

Theorem 1. *Assume that M_k and M_k^{-1} are uniformly bounded in norm. Then the sequence $\{\mu_j^{(k)}\}$ converges monotonically downward to λ_j.*

Proof. From (2) and the minimax theorem[1,8,13], we have

$$\mu_j^{(k+1)} = \min_{V_j} \max_{\substack{q \in V_j \\ q \neq 0}} \frac{q^T [X^{(k+1)^T} A X^{(k+1)}] q}{q^T [X^{(k+1)^T} X^{(k+1)}] q} \tag{6}$$

where V_j is a j dimensional subspace in $\mathbf{R^m}$. The eigenvalue problem for W_k can be written in

$$W_k y^{(k)} = \theta^{(k)} y^{(k)} \tag{7}$$

The eigenvalues are ordered as follows

$$\theta_1^{(k)} \leq \theta_2^{(k)} \leq \cdots \leq \theta_j^{(k)} \leq \cdots \leq \theta_n^{(k)} \tag{8}$$

By substituting $\mu_j^{(k)}$ and $X^{(k)}$ for $\mu_j^{(k+1)}$ and $X^{(k+1)}$ in (6), respectively, and applying lemma, we have

$$\mu_j^{(k)} \geq \lambda_i, i = 1, 2, \cdots, j \tag{9}$$

From the Sylvester's law of inertia[13] on W_k, we obtain

$$\theta_i^{(k)} \leq 0, i = 1, 2, \cdots, j \tag{10}$$

Let $U^{(k)}$ be a matrix formed by the orthonormal eigenvectors of W_k. Then

$$U^{(k)^T} W_k U^{(k)} = \begin{pmatrix} D_1^{(k)} & 0 \\ 0 & D_2^{(k)} \end{pmatrix} \tag{11}$$

where $D_1^{(k)} = diag(\theta_1^{(k)}, \cdots, \theta_m^{(k)})$, $U^{(k)} = [Y_1^{(k)}, Y_2^{(k)}]$, $Y_1^{(k)} \in \mathbf{R}^{n\times m}$ is the same as that in Step 4) of the PBL algorithm.

If z is an n dimensional nonzero vector of the following form

$$z = (z_1, \cdots, z_j, 0, \cdots, 0)^T = (v^T, 0^T)^T$$

where $v \in V_j$, then from (8) we have

$$z^T U^{(k)^T} W_k U^{(k)} z = \sum_{i=1}^{j} \theta_i^{(k)} z_i^2 \leq \theta_j^{(k)} \|v\|_2^2 \tag{12}$$

From (3), (4) and (12), we get

$$v^T (X^{(k+1)^T} A X^{(k+1)}) v - \mu_j^{(k)} v^T (X^{(k+1)^T} X^{(k+1)}) v \leq \theta_j^{(k)} \|v\|_2^2$$

Thus

$$\mu_j^{(k)} \geq \max_{\substack{v\in V_j \\ v\neq 0}} \left\{ \frac{v^T [X^{(k+1)^T} A X^{(k+1)}] v}{v^T [X^{(k+1)^T} X^{(k+1)}] v} - \frac{\theta_j^{(k)}}{v^T [X^{(k+1)^T} X^{(k+1)}] v / \|v\|_2^2} \right\}$$

In comparison with (6), we have

$$\mu_j^{(k)} \geq \mu_j^{(k+1)} + \min_{\substack{v\in V_j \\ v\neq 0}} \frac{(-\theta_j^{(k)})}{v^T [X^{(k+1)^T} X^{(k+1)}] v / \|v\|_2^2} \tag{13}$$

Then the sequence $\{\mu_j^{(k)}\}$ decreases monotonically. From (9) we have

$$\mu_j^{(k)} \geq \lambda_j$$

Hence the sequence $\{\mu_j^{(k)}\}$ has a limit τ, i.e.,

$$\mu_j^{(k)} \to \tau, (k \to \infty)$$

From (13), we have

$$\theta_j^{(k)} \to 0, (k \to \infty)$$

Then $\|W_k^{-1}\|$ goes to infinity. With

$$\|W_k^{-1}\| = \|L_k^T(A - \mu_j^{(k)}I)^{-1}L_k\| \le \|L_k^T\|\|(A - \mu_j^{(k)}I)^{-1}\|\|L_k\|$$

and the fact that $\|L_k\|$ and $\|L_k^T\|$ are bounded, $\mu_j^{(k)}$ must be converging to an eigenvalue of A. Since the j-th smallest eigenvalue of W_k converges to zero, it follows from the Sylvester's law of inertia that the j-th smallest eigenvalue of $A - \tau I$ is zero. Therefore we must have $\tau = \lambda_j$.

Let $\mu_j^{(k)}$ converge to λ_j. The next theorem shows that this convergence is asymptotically quadratic.

Theorem 2. *Assume that both M_k and M_k^{-1} are uniformly bounded in norm. Then the sequence $\{\mu_j^{(k)}\}$ converges to λ_j at an asymptotically quadratic rate.*

Proof. Let $\mu_j^{(k)} = \lambda_j + \epsilon^{(k)}$. It follows from (6) and the minimax theorem that there is an m dimensional vector $q = \tilde{q}^{(k)}$ such that

$$\mu_j^{(k+1)} = \frac{\tilde{q}^{(k)^T}[X^{(k+1)^T}AX^{(k+1)}]\tilde{q}^{(k)}}{\tilde{q}^{(k)^T}[X^{(k+1)^T}X^{(k+1)}]\tilde{q}^{(k)}} \tag{14}$$

Letting $X^{(k+1)}\tilde{q}^{(k)} = y^{(k)}$, we have

$$\mu_j^{(k+1)} = \mu_j^{(k)} + \frac{y^{(k)^T}(A - \mu_j^{(k)}I)y^{(k)}}{y^{(k)^T}y^{(k)}} = \mu_j^{(k)} + \frac{\alpha_j^{(k)}}{y^{(k)^T}y^{(k)}} \tag{15}$$

where $\alpha_j^{(k)} = y^{(k)^T}(A - \mu_j^{(k)}I)y^{(k)}$. It follows from the perturbation theory with respect to the eigenvectors of the symmetric matrix $A - \mu_j^{(k)}I$ [1] that there is a bounded scalar $\beta^{(k)}$ such that , when k is sufficiently large, $y^{(k)}$ can be written as (within a scalar factor)

$$y^{(k)} = x_j + \beta^{(k)}\epsilon^{(k)}s_j \tag{16}$$

where x_j is a null vector of the matrix $A - \lambda_j I$ and the vector s_j is orthogonal to the null space of $A - \lambda_j I$ with $\|s_j\|_2 = 1$. Then

$$\left\{ \begin{array}{l} \alpha_j^{(k)} = y^{(k)^T}(A - \lambda_j I)y^{(k)} - \epsilon^{(k)}y^{(k)^T}y^{(k)} = -\epsilon^{(k)}y^{(k)^T}y^{(k)} + O(\epsilon^{(k)^2}) \\ y^{(k)^T}y^{(k)} = \|x_j\|_2^2 + O(\epsilon^{(k)}) \end{array} \right. \tag{17}$$

From (15) and (17), we have

$$\mu_j^{(k+1)} = \mu_j^{(k)} - \epsilon^{(k)} + O(\epsilon^{(k)^2}) = \lambda_j + O(\epsilon^{(k)^2})$$

Thus

$$\epsilon^{(k+1)} = O(\epsilon^{(k)^2})$$

and we have quadratic convergence.

4. Implementation and Numerical Experiments

We first discuss some implementation details of the PBL algorithm. The main cost of the PBL algorithm is in the block Lanczos loop. The early termination test in Step 4) of the PBL algorithm can reduce the number of block Lanczos iterations. To avoid solving the generalized eigenvalue problem (2), we can use the modified Gram-Schmidt process to orthonormalize the matrix $X^{(k)}$. The symbol MGS denotes the modified Gram-Schmidt algorithm. Then the PBL algorithm can be modified as follows.

Modified PBL Algorithm. Choose an integer $m (m \geq j)$ and an orthonormal matrix $X^{(0)} \in \mathbf{R}^{n \times m}$.

For $k = 0, 1, \cdots$, do 1) to 6)

1) Compute $A_k = X^{(k)^T} A X^{(k)}$, find the j smallest eigenvalues $\mu_1^{(k)}, \cdots, \mu_j^{(k)} (\mu_1^{(k)} \leq \cdots \leq \mu_j^{(k)})$ and corresponding eigenvectors $q_1^{(k)}, \cdots, q_j^{(k)}$ of the matrix A_k of order m, and let $Q^{(k)} = [q_1^{(k)}, \cdots, q_j^{(k)}]$.

2) Choose M_k to be a symmetric positive definite matrix approximating $A - \mu_j^{(k)} I$, and compute the Cholesky factorization $M_k = L_k L_k^T$.

3) Define the matrix $W_k = L_k^{-1}(A - \mu_j^{(k)} I) L_k^{-T}$.

4) $V_k = MGS(L_k^T X^{(k)} Q^{(k)})$.

5) Run the block Lanczos algorithm with W_k and starting orthonormal matrix V_k until the j-th smallest Ritz value converges. Letting $\theta_1^{(k)}, \cdots, \theta_j^{(k)}, \cdots, \theta_m^{(k)} (\theta_1^{(k)} \leq \cdots \leq \theta_m^{(k)})$ and $y_1^{(k)}, \cdots, y_j^{(k)}, \cdots, y_m^{(k)}$ be the m smallest Ritz values and corresponding unit Ritz vectors of W_k, this stopping test is $\|W_k y_j^{(k)} - \theta_j^{(k)} y_j^{(k)}\|_2 < \epsilon$. Let $Y_1^{(k)} = [y_1^{(k)}, \cdots, y_m^{(k)}]$.

6) Let $X^{(k+1)} = MGS(L_k^{-T} Y_1^{(k)})$.

Remark 4.1. If we denote by $\hat{A}_k$ the linear transformation defined by $\hat{A}_k = P_k A P_k$ where P_k is an orthogonal projector onto $span(X^{(k)})$, then the matrix A_k represents the restriction of the operator $\hat{A}_k$ to the subspace $span(X^{(k)})$. Therefore, the eigenvalue problem for the matrix A_k is the Rayleigh-Ritz procedure of the matrix A with respect to the orthonormal basis $X^{(k)}$ of the subspace $span(X^{(k)})$. The Rayleigh-Ritz procedure is used in the outside loop of both the PBL algorithm and the modified PBL algorithm, while the difference between the two algorithms is only the choice of the used basis. So the modified PBL algorithm has the same convergence results as the PBL algorithm.

Remark 4.2. On the choice of preconditioner, Morgan and Scott's discussion[19] is suitable for the modified PBL algorithm.

Remark 4.3. If the p smallest eigenpairs are desired, then we may let the modified PBL algorithm run for j going from 1 until p (let $m \geq p$).

Now we briefly report some of our numerical experiments with the modified PBL algorithm. Comparisons are made with the block Lanczos method. All tests were made on IBM-AIX/UNIX at the University of Calgary. Double precision arithmetic was used throughout. The p smallest eigenvalues and corresponding eigenvectors are computed. $\|r_i^{(k)}\|_2$ denotes the residual norm $\|AX^{(k)}q_i^{(k)} - \mu_i^{(k)}X^{(k)}q_i^{(k)}\|_2 (i = 1, \cdots, p)$. The requested residual tolerance for the j-th smallest eigenpair is 10^{-8}.

Example 4.1[19]. The first matrix $A = diag(1, 2, 3, \cdots, 1000)$. Let $p = 4$ and $m = 8$. The 1000×8 initial orthonormal matrix is randomly chosen. For the preconditioner, let $M = diag(10.1, 10.2, \cdots, 110)$ and $M_k = M - \mu_p^{(k)}I$. Table 4.1 gives the results of the modified PBL algorithm. It lists the number of iterations in the block Lanczos loop. The size of the Krylov subspace generated by the block Lanczos method is fixed on 30. It shows the expected quadratic convergence. The total number of block Lanczos iterations is 36. The block Lanczos algorithm requires 215 iterations for the same task. So the modified PBL algorithm reduces greatly the number of iterations of the block Lanczos algorithm.

Table 4.1 Modified PBL algorithm for Example 4.1

k	block Lanczos iterations	$\lvert\lambda_1 - \mu_1^{(k)}\rvert$	$\lvert\lambda_2 - \mu_2^{(k)}\rvert$	$\lvert\lambda_3 - \mu_3^{(k)}\rvert$	$\lvert\lambda_4 - \mu_4^{(k)}\rvert$
0		0.4493E+03	0.4682E+03	0.4869E+03	0.4910E+03
1	1	0.5887E+01	0.6507E+01	0.9284E+02	0.9611E+01
2	5	0.1160E+00	0.1740E+01	0.1927E+01	0.1818E+01
3	1	0.1420E-01	0.1003E+01	0.7546E+00	0.8132E-02
4	2	0.1238E-04	0.2055E-02	0.1074E-03	0.6897E-05
5	12	0.4793E-11	0.5584E-09	0.7328E-09	0.3156E-10
6	15	0.0000E+00	0.1487E-20	0.5310E-19	0.8231E-21

If the smallest eigenpair is only computed, M is as above defined. Let $m = p = 1$. The starting vector is $(1, 1/2, 1/3, \cdots, 1/1000)^T$ (see [19]). Table 4.2 gives the results of the modified PBL algorithm for $m = p = 1$ (The size of the Krylov subspace generated by the iterative Lanczos method is fixed on 16). The results are better than those[19].

Table 4.2 Modified PBL algorithm for Example 4.1 and $m = p = 1$

k	Lanczos iterations	$\mu_1^{(k)}$	residual norm
0		0.4553387350E+01	0.2424E+02
1	1	0.1000087654E+01	0.6251E-01
2	2	0.1000000000E+01	0.1984E-04
3	2	0.1000000000E+01	0.7940E-08

Next we compare the modified PBL algorithm with the block Lanczos method. Let $A = diag(1, 1 + \delta, 1 + 2\delta, \cdots, 1 + 99\delta, 2 + 99\delta, \cdots, 901 + 99\delta)$, for $\delta = 1, 0.1$ and 0.01. Three matrices with increasing difficulty are used. The 4 smallest eigenvalues and corresponding eigenvectors are computed. Let $m = 8$ and $M = diag(1.1, 1.2, 1.3, \cdots, 101)$, and the preconditioner $M_k = M - \mu_j^{(k)}I$. The initial matrices for the modified PBL algorithm and the block Lanczos method are randomly chosen in same way. Table 4.3 gives the total number of matrix-vector products and the time in CPU seconds used for each of two methods. For the toughest problems ($\delta = 0.01$), the modified PBL algorithm is much better than the block Lanczos method.

Table 4.3 Comparison between the modified PBL algorithm and the block Lanczos method for Example 4.1

Method	Number of matrix-vector products			CPU time (second)		
	matrix $\delta = 1$	matrix $\delta = 0.1$	matrix $\delta = 0.01$	matrix $\delta = 1$	matrix $\delta = 0.1$	matrix $\delta = 0.01$
Modified PBL algorithm	1120	280	1360	93.4	26.4	109.2
Block Lanczos method	4246	31965	278843	331.6	2505.8	20847.7

Example 4.2. We consider the matrix $A = diag(0, 0, 0.05, 0.05, 0.05, 0.06, \cdots, 0.01 \times i, \cdots, 18)$. The 2 smallest eigenvalues and corresponding eigenvectors are computed. Let $m = 6$, $M = diag(1.1, 1.2, 1.3, \cdots, 181)$ and the preconditioner $M_k = M - \mu_2^{(k)} I$. The initial matrix is randomly chosen. Table 4.4 gives the results of the modified PBL algorithm.

Table 4.4 Modified PBL algorithm for Example 4.2

k	block Lanczos Method	Ritz values		residual norm	
		$\mu_1^{(k)}$	$\mu_2^{(k)}$	$\Vert r_1^{(k)}\Vert_2$	$\Vert r_2^{(k)}\Vert_2$
0		0.8520202362E+01	0.8616998218E+01	0.5319E+01	0.5146E+01
1	1	0.7118714290E+00	0.7699999932E+00	0.3659E+00	0.2758E+00
2	1	0.2925016104E-05	0.1683996736E-02	0.2478E-02	0.3252E-01
3	1	0.5136305635E-10	0.4706634886E-07	0.7629E-05	0.2557E-03
4	2	0.6629452670E-19	0.1465064694E-15	0.2682E-09	0.1329E-07
5	1	0.3156949816E-23	0.1032346310E-19	0.2248E-11	0.1305E-09

For the example, it is impossible to find the double eigenvalue zero by using the PL algorithm. Table 4.5 gives the total number of matrix-vector products and the time in CPU seconds used for the modified PBL algorithm and the block Lanczos method.

Table 4.5 Comparison between the modified PBL algorithm and the block Lanczos method for Example 4.2

Method	Number of matrix-vector products	CPU time (second)
Modified PBL algorithm	120	7.8
Block Lanczos method	2730	208.3

Example 4.3. Consider the matrix of order 2500 defined as

$$A = \frac{1}{h^2}\begin{pmatrix} B & -I & & & 0 \\ -I & B & -I & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot \quad \cdot & -I \\ 0 & & & -I & B \end{pmatrix}, B = \begin{pmatrix} 4 & -1 & & & 0 \\ -1 & 4 & -1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot \quad \cdot & -1 \\ 0 & & & -1 & 4 \end{pmatrix}, h = 1/51$$

which is derived from five-point discrete approximation to the second-order selfadjoint elliptic partial differential equation

$$-\frac{\partial^2 u(x,y)}{\partial x^2} - \frac{\partial^2 u(x,y)}{\partial y^2} = \lambda u(x,y)$$

with the boundary condition $u(x,y)|_\Gamma = 0$, where Γ denotes the boundary of the square region $\mathbf{R} = \{(x,y)|0 \le x \le 1, 0 \le y \le 1\}$. The 5 smallest eigenvalues of the matrix A are 19.7329678198, 49.2949925965, 49.2949925965, 78.8570173732 and 98.4404193543.

The 4 smallest eigenpairs are computed. Let $m = 8, p = 4$. The preconditioner is from incomplete factorization of $A - \mu_j^{(k)} I$ (see [16]). Table 4.6 gives the total number of matrix-vector products with A, along with the time in CPU seconds used for the modified PBL algorithm and the block Lanczos method.

Table 4.6 Comparison between the modified PBL algorithm and the block Lanczos method for Example 4.3

Method	Number of matrix-vector products	CPU time (second)
Modified PBL algorithm	780	158.6
Block Lanczos method	4018	804.9

5. Conclusions

The modified PBL algorithm is a generalization of the PL algorithm, and uses preconditioning to accelerate the convergence of the block Lanczos method. A double iteration scheme is used. The Rayleigh-Ritz procedure and preconditioning are applied in the outside loop; the block Lanczos method is used in the inner loop. The inner iteration is terminated early for efficiency, but convergence is still asymptotically quadratic with respect to the outer loop. The modified PBL algorithm can significantly reduce the expense of computing eigenpairs of some sparse matrices. It is one of the most efficient methods for difficult problems with close or multiple eigenvalues.

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