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A method for determining intermediate eigensolutions of large, sparse, symmetric matrices by the double shifted inverse power method in the generalized eigenvalue problem

by
Mitsuhiro KASHIWAGI *

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Abstract

The inverse power method is often used to solve large, sparse and symmetric eigenproblems. This paper presents a useful method on the double shifted inverse power method in the eigensolution of large sparse and symmetric matrices. The proposed method is a method requiring only a relatively small computational time which has the good accuracy and stability. The results obtained agree well with the exact solutions in short CPU time and this indicates that the proposed method provides efficient convergency.

1. INTRODUCTION

Numerical simulations in computational dynamics or other fields are often reduced to linear equations or eigenvalue problems with large, sparse and symmetric matrices. These are usually solved with preconditioned iterative conjugate gradient (PCG) methods such as incomplete Cholesky conjugate gradients (ICCG) and scaled conjugate gradients (SCG), combined with algebraic multigrid (AMG) preconditioners [1,2,4,7,12,13]. Because these require much less use of the main storage area in memory, they have proven to be more powerful analytical approaches for the large sparse symmetric matrices created using the finite element method (FEM). Still, eigenvalue analysis is an ill-conditioned numerical method employing determinant of a matrix with zero, and so solution methods dependent on diagonally dominant matrices such as AMG and ICCG are not very effective for identifying intermediate eigenvalues. To make use of the sparsity of the matrices appearing in large, sparse and symmetric eigenvalue problems such as FEM, one must employ iterative methods such as power method solvers or Lanczos solvers [2,3,5,6,9,10, 11,14,15]. However, none of these solutions, except the inverse power method, is effective for finding intermediate eigenvalues.

Iterative methods such as the inverse power method, the subspace methods and the restart Lanczos method [2] are effective for finding intermediate eigenvalues after the minimum or maximum eigenvalue is identified [9,10,11], but they present insoluble or overlooked intermediate eigensolutions in the vicinity of the shifted origin. Because there is no appropriate way to calculate intermediate eigenvalues, the current approach is to start with the minimum and calculate “up” some hundreds or thousands of eigenvalues. This kind of analysis imposes an immense calculation load, and is only considered efficient for calculating some tens (at most) of the eigensolutions in the neighborhood of any one known eigenvalue.

Moving the origin to the neighborhood of an eigenvalue to search for more eigenvalues is called the *shifted origin inverse power method*. Once the shift distance is set correctly, we can expect calculations to converge more quickly than they would if the origin had been left in its original position. It is a classic

* Professor,
Department of Architecture, School of Industrial Engineering,
Tokai University

approach, but the iterative shifted origin inverse power method appears to be the only effective method for eigenvalue analysis in the vicinity of the shifted origin, especially for arbitrarily selected intermediate locations for the shifted origin. However, the matrices for eigenvalues approximately midway between the minimum and the maximum eigenvalues are particularly ill-conditioned, forcing extremely high numbers of iterations and long calculation times. Solving ill-conditioned linear equations is a difficult problem by itself; it is hard to reduce the number of iterations in PCG. Consequently, it is desirable to find a way to reduce the number of iterations in the shifted origin inverse power method.

This paper proposes a method to find intermediate eigensolutions in the vicinity of a shifted origin in a large sparse symmetric matrix. The shifted origin is held stationary at its new location in the conventional shifted origin inverse power method. In this method, however, when the relative residual error of the just-determined eigenvalue is above some convergence value, the conventional shifted origin inverse power method (here, designated the simultaneous shifted inverse power method) is employed. Once the relative residual error falls below the threshold, the shift distance is reset at every iteration of the shifted origin inverse power method (here, designated the consecutive shifted inverse power method). This enables the algorithm to reach a solution in approximately half the number of iterations and half the time of the conventional shifted origin inverse power method (here, designated the double shifted inverse power method). An appropriate shift distance affects the number of iterations and calculation time to convergence, so this approach is also proposed for setting the shift distance in general eigenvalue problems. With the inverse power method, the eigenvalues near the origin are solved in order from the eigenvalue with the value nearest to the eigenvalue used for shifting the origin. This approach is effective when finding multiple intermediate eigensolutions in a large, sparse and symmetric matrix with a preconditioned iterative method such as SCG. Another advantage of this approach is that it can be used to search for solutions from the maximum eigenvalue downward, as well as from the minimum one upward. However, one cannot guarantee that an eigensolution that has been “identified” with the inverse power method is genuine, so one must “identify” more solutions than one actually needs and then eliminate the false solutions. The proposed method also reduces the number of identifications required for this process.

The following describes the theory behind determining the consecutive shift point and the algorithm. Numerical experiments with three-dimensional (3D) Helmholtz problems in the standard eigenvalue problem and plane frame problems in the generalized eigenvalue problem are carried out, as these often have multiple roots. This method is shown to be effective.

2. SHIFT DISTANCE FOR THE ORIGIN

The following general eigenvalue problem is handled here:

$$Ax = \lambda Bx \qquad (1)$$

where A is a real symmetric $n \times n$ matrix, B is a positive $n \times n$ definite symmetric matrix, λ is the eigenvalue, and x is the eigenvector corresponding to the eigenvalue.

A well-chosen origin shift distance λ_0 enables speedy convergence to a low-order eigenvector. When an approximate value for the eigenvalue is already known, shifting the origin near to that value will speed convergence on the eigenvectors corresponding to nearby eigenvalues. Generally, it is rare for an approximate value to be known beforehand for an eigenvalue. The Rayleigh quotient of an approximate eigenvector obtained during iteration and the norm of the corresponding residual vector are used to estimate the limits of the domain of the eigenvalue. The origin is then shifted to the interior of that domain. The procedure is as follows.

If the B-orthogonalized eigenvectors corresponding to the eigenvalues $\lambda_{\mathrm{i}}\left(1 \le i \le n\right)$ are written as $\phi_i\left(1 \le i \le n\right)$, the eigenvector x is decomposed into an eigenspace. If we denote the coefficient for each ϕ_i as c_i, we can write

$$x = \sum_{i=1}^{n} c_i \phi_i \qquad (2)$$

Then, we have

$$x^T A x = \sum c_j \phi_j A \sum c_i \phi_i = \sum_{i=1}^{n} \lambda_i c_i^2 \qquad (3)$$

Using

$$x^T Bx = 1 \qquad (4)$$

we obtain

$$x^T Bx = \sum_i c_i \phi_i B \sum_j c_j \phi_j = \sum_i c_i^2 = 1 \qquad (5)$$

Accordingly,

$$x^T Ax = \sum_{i=1}^{n} x^T Axc_i^2 \qquad (6)$$

$$A\phi_i = \lambda_i B\phi_i$$

and from Eq. (2), we find

$$Ax = \sum c_i A\phi_i = \sum c_i \lambda_i B\phi_i$$

$$x^T AB^{-1}Ax = \sum c_j \lambda_j \phi_j BB^{-1} \sum c_i \lambda_i B\phi_i = \sum c_i^2 \lambda_i^2 \qquad (7)$$

From Eqs.(3) and (6), we know that

$$\sum_{i=1}^{n} (x^T Ax - \lambda_i)c_i^2 = 0$$

Therefore,

$$\begin{aligned}
\sum (x^T Ax - \lambda_i)^2 c_i^2 &= \sum \left\{ \left(x^T Ax\right)^2 - 2x^T Ax\lambda_i + \lambda_i^2 \right\} c_i^2 \\
&= \sum (x^T Ax)^2 c_i^2 - 2\sum x^2 Ax\lambda_i {c_i}^2 + \sum {\lambda_i}^2 {c_i}^2 \\
&= (x^T Ax)^2 \sum {c_i}^2 - 2x^T Ax \sum \lambda_i c_i^2 + \sum \lambda_i^2 c_i^2 \\
&= (x^T Ax)^2 x^T Bx - 2x^T Ax \cdot x^T Ax + x^T AB^{-1} Ax \\
&= (x^T Ax \cdot Bx - Ax)^T (x^T Ax \cdot x - B^{-1} Ax) \\
&= (x^T Ax \cdot Bx - Ax)^T B^{-1} (x^T Ax \cdot Bx - Ax) \\
&= r^T B^{-1} r \qquad (8)
\end{aligned}$$

where $r = x^T Ax \cdot Bx - Ax$.

It follows that there exists a scalar ρ for

$$\left| x^T Ax - \lambda_j \right| {c_j}^2 \le \sum_{i \ne j} \left| x^T Ax - \lambda_i \right| {c_i}^2$$

$$\le \frac{1}{\rho} \sum_{i=1}^{n} \left[x^T Ax - \lambda_i \right]^2 {c_i}^2 = \frac{1}{\rho} r^T B^{-1} r \qquad (9)$$

Furthermore, from

$$r^T \cdot B^{-1} r = \sum \left[x_i - x^T Ax \right]^2 {c_i}^2 \ge \rho^2 \sum {c_i}^2 \ ,$$

we know that

$${c_j}^2 = 1 - \sum_{i \ne j} {c_i}^2 \ge 1 - \frac{r^T B^{-1} r}{\rho^2}$$

From this, we obtain

$$\left| x^T Ax - \lambda_j \right| \le \frac{1}{{c_j}^2} \frac{r^T B^{-1} r}{\rho} \le \frac{\dfrac{r^T B^{-1} r}{\rho}}{1 - \dfrac{r^T B^{-1} r}{\rho^2}} = \frac{\rho \cdot r^T B^{-1} r}{\rho^2 - r^T B^{-1} r} \qquad (10)$$

Generally, when the relationship given in Eq. (11) holds between the Rayleigh quotient $\lambda(x)$ and any eigenvalue λ_i , Eq. (12) also holds:

$$\left| \lambda(x) - \lambda_i \right| \ge \rho > 0 \qquad (11)$$

$$\left| \lambda(x) - \lambda_i \right| \le \beta \ , \ \beta = \frac{\rho \cdot r^T B^{-1} r}{\rho^2 - r^T B^{-1} r} \ , \ j \ne i \qquad (12)$$

In the inverse power method, the following simultaneous linear equations will be solved at the time of repetition.

$$[A - \lambda_0 B]x = b \qquad (13)$$

where x is the approximation eigenvector before solving the equation (13).

The quadratic form of a matrix $A - \lambda_0 B$ is expressed as follows:

$$f = x^T \left[A - \lambda_0 B \right] x$$

The upper formula is as follows.

$$f = x^T b = b^T [A - \lambda_0 B]^{-1} b = b^T \sum_{i=1}^{n} \frac{\phi_i \phi_i^T}{\lambda_i - \lambda_0} b = \sum_{i=1}^{n} \frac{(b^T \phi_i)^2}{\lambda_i - \lambda_0} \qquad (15)$$

in which ϕ_i is the i -th eigenvector, where $i = 1$ denotes the smallest eigenvalue.

When $\lambda_0 < \lambda_l$ and $f > 0$, that is $A - \lambda_0 B$ is a positive definite matrix. On the other hand, when $\lambda_0 > \lambda_l$ and $f < 0$, that is $A - \lambda_0 B$ is non-positive definite.

The following expressions expect decreasing the number of iteration of the inverse power method and shortening at the computing time when the approximation eigenvalue by the Rayleigh quotient is almost near a true eigenvalue.

$$r_i^{(m)} = Ax_i^{(m)} - \lambda_i^{(m)} Bx_i^{(m)} \qquad (16)$$

$$\rho_i^{(m)} = \left| \lambda_i^{(m)} - \lambda_i^{(m-1)} \right| \qquad (17)$$

$$\beta_i^{(m)} = \frac{\rho_i^{(m)} \cdot r_i^{(m)T} B^{-1} r_i^{(m)}}{\left(\rho_i^{(m)}\right)^2 - r_i^{(m)T} r_i^{(m)}} \qquad (18)$$

$$\lambda_0^{(m+1)} = \lambda_i^{(m)} - sign\left(x_i^{(m)T} x_i^{(m-1)}, x_i^{(m-1)T} x_i^{(m-2)} \right) \beta_i^{(m)} \qquad (19)$$

in which ${\lambda_i}^{(m)}$ is the Rayleigh quotient of the approximate eigenvector ${x_i}^{(m)}$ in m iteration for the eigenvalue $\lambda_{\mathrm{i}} \ (1 \le i \le n)$ of the real symmetrical matrix A .

3. ALGORITHM FOR THE DOUBLE SHIFTED INVERSE POWER METHOD

Let us assume that A is a stiffness matrix, B is a mass matrix, λ is an eigenvalue, and x is an eigenvector. In the general eigenvalue problem, when the origin is shifted by the distance λ_0 , it is expressed as $\left[A - \lambda_0 B \right] x = (\lambda - \lambda_0) Bx$. The algorithm for the double shifted inverse power law method is shown here for the general eigenvalue problem.

(1) $\ell = 0$

The initial vector $x^{(0)}$ is generated using uniform random numbers. The Gram-Schmidt algorithm is used to select and normalize previously obtained eigenvectors.

$$\widetilde{x}^{(0)} = x^{(0)} - \sum_{j=1}^{i} ({x^{(0)}}^T B\phi_j)\phi_j \quad , \quad x^{(0)} = \widetilde{x}^{(0)} \Big/ ({\widetilde{x}^{(0)}}^T B\widetilde{x}^{(0)})^{\frac{1}{2}} \quad ,$$

$$\lambda^{(0)} = {x^{(0)}}^T A x^{(0)}$$

(2) $\ell = 1,\ 2,\ \cdots$

Iteration is performed with the simultaneous shifted inverse power method.

① At cycle ℓ , $x^{(\ell)}$ is found using

$x^{(\ell)} = \left[A - \lambda_0 B\right]^{-1} B\, x^{(\ell-1)}$. The Gram-Schmidt algorithm is used to select and normalize previously obtained eigenvectors. The approximate eigenvalue is calculated using the Rayleigh quotient.

$$\widetilde{x}^{(\ell)} = x^{(\ell)} - \sum_{j=1}^{i} \left({x^{(\ell)}}^T B\phi_j\right)\phi_j \quad , \quad x^{(\ell)} = \widetilde{x}^{(\ell)} \Big/ ({\widetilde{x}^{(\ell)}}^T B\widetilde{x}^{(\ell)})^{\frac{1}{2}} \quad ,$$

$$\lambda^{(\ell)} = {x^{(\ell)}}^T A x^{(\ell)}$$

② The shift distance $\lambda_0^{(k)}$ is selected when

$\left| \dfrac{\lambda^{(\ell)} - \lambda^{(\ell-1)}}{\lambda^{(\ell)}} \right| < \varepsilon_e$. If this condition is not satisfied, return to ① in (2). In unique models with many multiple roots and roots extremely close to each other in value, ε_e is the relative error of the eigenvalue at the simultaneous shift as followings.

$$\varepsilon_e = \min\left(10^{-3} / (\lambda_0 + 1), 10^{-7}\right) \tag{29}$$

or

$$\varepsilon_e = \min\left(10^{-4} / (\lambda_0 + 1), 10^{-7}\right) \tag{30}$$

In standard models free from many multiple roots and roots extremely close to each other in value, ε_e is the relative error of the eigenvalue at the simultaneous shift as followings.

$$\varepsilon_e = \min\left(10^{-1} / (\lambda_0 + 1), 10^{-5}\right) \tag{31}$$

(3) $m = 1,\ 2,\ \cdots$

Iteration is performed with the consecutive shifted inverse power law method.

① At cycle m , $x^{(m)}$ is found using

$x^{(m)} = \left[A - \lambda_0^{(m)} B\right]^{-1} Bx^{(m-1)}$. The Gram-Schmidt algorithm is used to select and normalize previously obtained eigenvectors. The approximate eigenvalue is calculated using the Rayleigh quotient.

$$\widetilde{x}^{(m)} = x^{(m)} - \sum_{j=1}^{i} \left({x^{(m)}}^T B\phi_j\right) \phi_j \ ,$$

$$x^{(m)} = \widetilde{x}^{(m)} \Big/ ({\widetilde{x}^{(m)}}^T B\widetilde{x}^{(m)})^{\frac{1}{2}} \quad , \quad \lambda^{(m)} = {x^{(m)}}^T A x^{(m)}$$

□Convergence is tested with $\left| \dfrac{\lambda^{(m)} - \lambda^{(m-1)}}{\lambda^{(m)}} \right| < \varepsilon_1 = 1 \times 10^{-14}$. Or, the residual vector $r^{(m)} = A\, x^{(m)} - \lambda^{(m)} B\, x^{(m)}$ is calculated and if $\dfrac{\left\| r^{(m)} \right\|}{\left\| A\, x^{(m)} \right\|} < \varepsilon_2 = 1 \times 10^{-9}$ then convergence is assumed. If the calculation has not converged, calculate $\lambda_0^{(m)}$ using the following equation, and return to ① in (3).

$$e = \left|\lambda^{(m)} - \lambda^{(m-1)}\right| , \quad g = \left\{ r^{(m)} \right\}^T B^{-1} r^{(m)} , \quad \beta^{(m)} = eg / \left(e^2 - g\right) ,$$

$$\lambda_0^{(m+1)} = \lambda^{(m)} - sign\left({x^{(m)}}^T x^{(m-1)}, {x^{(m-1)}}^T x^{(m-2)} \right) \beta^{(m)} \tag{32}$$

In the standard eigenvalue problem, $B = I$.

4. NUMERICAL EXPERIMENT

A numerical experiment was carried out with some typical eigenvalue problems to validate the functionality of the double shifted inverse power method. The coefficient matrices for discretized Helmholtz equations occurring in steady problems of 3D wave equations and the plane frame problem were employed. Because the analytical solutions for these eigenvalue problems are known, they are useful for validating the accuracy of the eigenvalues provided by the numerical solution. These problems are also known for containing many multiple roots and roots extremely close to each other in value. The degree of freedom, origin shift distance and relative error at the simultaneous shift were varied. An iterative method (SCG) was employed to solve the resulting simultaneous equation. Many-dimensional sparse matrices are effective in the iterative method provided by pre-processing with ICCG or SCG, but ICCG showed instable conditions in calculations of the intermediate eigensolutions and required more calculation time than SCG, so the description of ICCG processing is omitted here. A key feature of the proposed method is that, although it begins with the greatest eigensolution and proceeds “downward”, opposite to the order of eigensolutions in the inverse power method, it can be applied in numerical analyses such as the inverse power method. However, it is not guaranteed under this method that all eigensolutions “identified” are in fact genuine, so a certain excess number of solutions must be sought in order to obtain the desired number of genuine solutions. This report also proposes the specific number of extra eigensolutions that must be found. This study does not assume access to a supercomputer; and so the authors deliberately used a typical PC of recent vintage from E machines (Windows XP Pentium 4, 2.8 GHz, 1536 MB of RAM, Fujitsu Fortran & C Academic package V4.0L10).

4.1 Standard Eigenvalue Problem (3-dimensional Helmholz Problem)

This section is concerned with a standard eigenvalue problem derived from a discretized 3-dimensional Helmholz problem defined on a rectangular domain. Centered-differences were used in the discretization, and upon fixing the value of the solution to be 0 everywhere on the boundary, a standard eigenvalue problem $A x = \lambda x$ is derived, where $A = [a_{k,l}]$ and each element of A is defined as follows:

$$a_{l,l} = \frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} + \frac{2}{\Delta z^2}, l = (k-1)n_x n_y + (j-1)n_x + i,$$

$$(1 \le i \le n_x, 1 \le j \le n_y, 1 \le k \le n_z),$$

$$a_{l,l+1} = a_{l+1,l} = -\frac{1}{\Delta x^2}, l = (k-1)n_x n_y + (j-1)n_x + i,$$

$$(1 \le i \le n_x, 1 \le j \le n_x, 1 \le k \le n_z),$$

$$a_{l,l+nx} = a_{l+n\times,l} = -\frac{1}{\Delta y^2}, l = (k-1)n_x n_y + (j-1)n_x + i,$$

$$(1 \le i \le n_x, 1 \le j \le n_y, 1 \le k \le n_z),$$

$$a_{l,l+nx\times ny} = a_{l+nx\times ny,l} = -\frac{1}{\Delta z^2}, l = (k-1)n_x n_y + (j-1)n_x + 1,$$

$$(1 \le i \le n_x, 1 \le j \le n_y, 1 \le k \le n_z),$$

$a_{l,m} = 0,\quad l,m$ except for the superscription,

where $n_x + 1$, $n_y + 1$ and $n_z + 1$ are nodal numbers in the *x, y* and z directions respectively, and l_x, l_y and l_z are the lengths of the domain in the *x, y* and z directions respectively, with $\Delta x = l_x/(n_x+1)$, $\Delta y = l_y/(n_y+1)$ and $\Delta z = l_z/(n_z+1)$. (Cf. Fig.1.) The analytical solution for this coefficient matrix A is given by the following equation:

$$\lambda_{i,j,k} = \frac{2}{\Delta x^2}\left(1-\cos\frac{i\pi}{n_x+1}\right) + \frac{2}{\Delta y^2}\left(1-\cos\frac{j\pi}{n_y+1}\right)$$

$$+\frac{2}{\Delta z^2}\left(1-\cos\frac{k\pi}{n_z+1}\right)$$

Table 1 shows the parameters $l_x, l_y, l_z, n_x, n_y, n_z$ and $n = n_x \times n_y \times n_z$ used in this experiment. Double precision arithmetic is used for all numerical calculations. The number of eigensolutions sought is $l = 1 \sim 20$. The initial vector is specified at random.

Figures 2 – 3 show the maximum values of the incorrect answers in all the models. If Eq. (29) is used for calculation of the relative error at a simultaneous shift, at most four incorrect answers exist in the 3D model; using Eq. (30) for the calculation, there is at most one value each in the 3D model.

Table 1. Parameters of the space model

model	type	l_x	l_y	l_z	n_x	n_y	n_z	n
A	A-1	1	1	1	16	16	16	4096
	A-2	1	1	1	22	22	22	10648
	A-3	1	1	1	28	28	28	21952
	A-4	1	1	1	34	34	34	39304
	A-5	1	1	1	40	40	40	64000

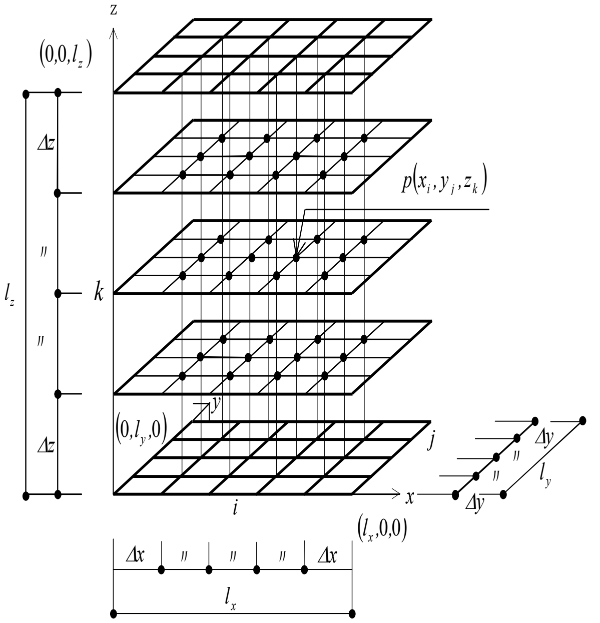

Figure 1. A space model for the standard eigenvalue problem

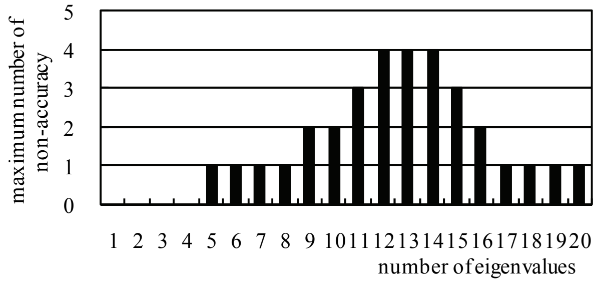

Figure 2. Maximum number of non-accuracy (space model, Eqs.(29))

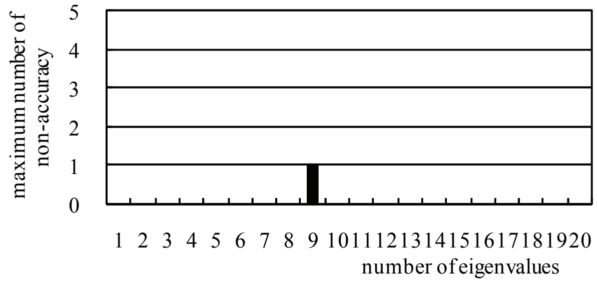

Figure 3. Maximum number of non-accuracy (space model, Eqs.(30))

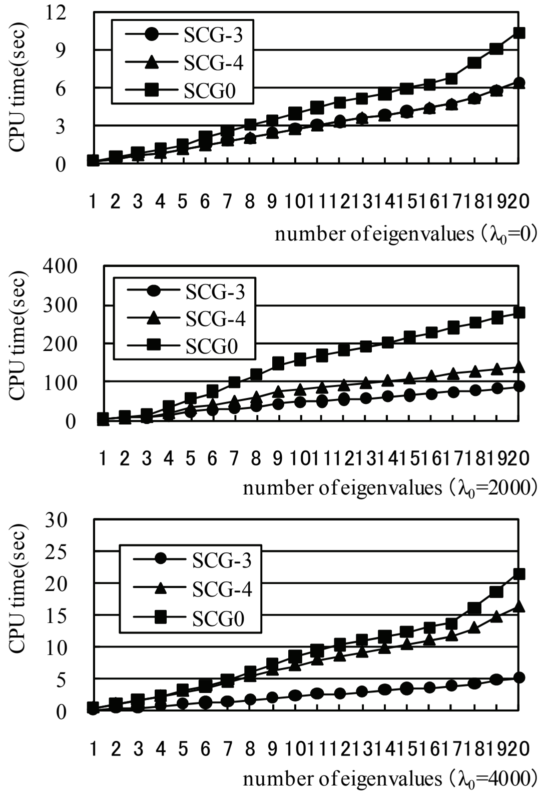

Figure 4. Computing time (space model, type A-1)

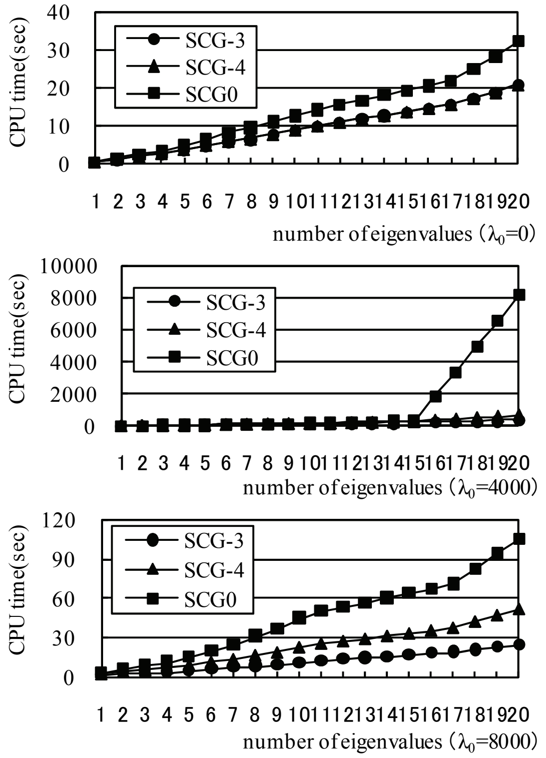

Figure 5. Computing time (space model, type A-2)

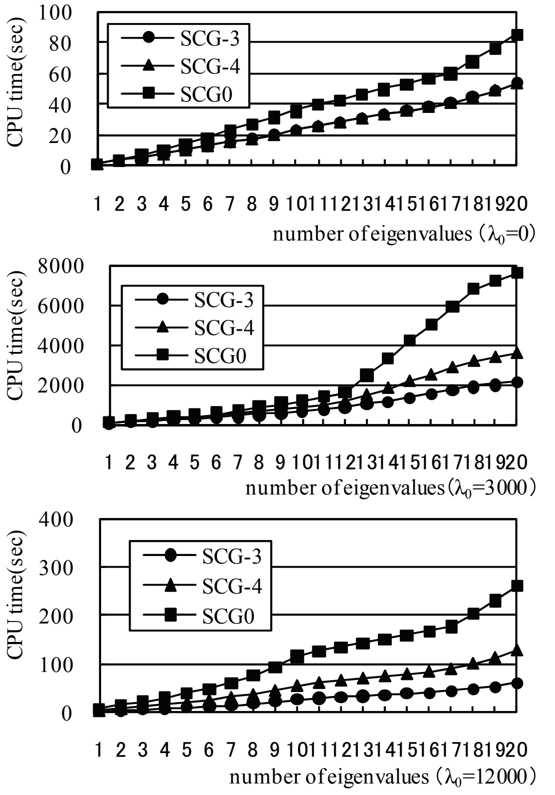

Figure 6. Computing time (space model, type A-3)

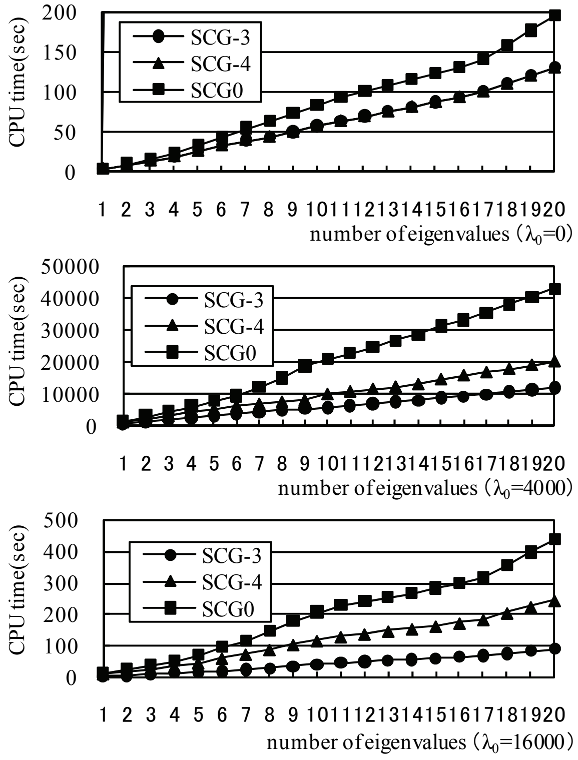

Figure 7. Computing time (space model, type A-4)

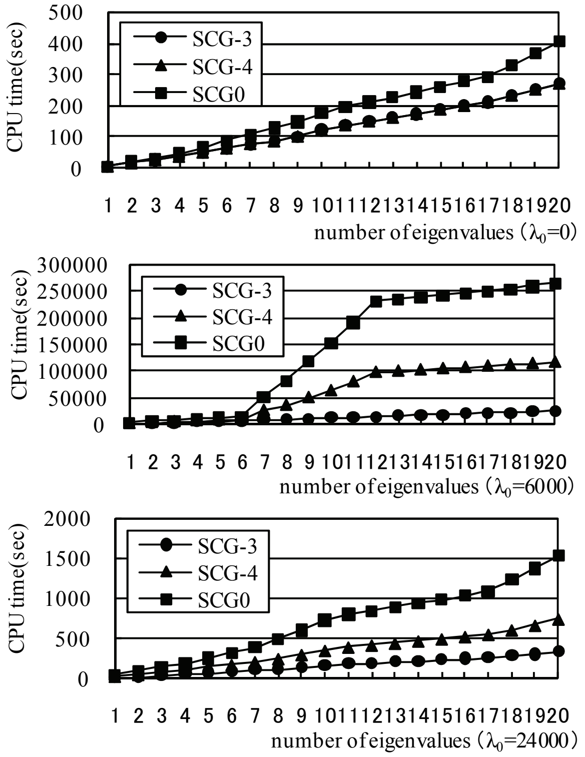

Figure 8. Computing time (space model, type A-5)

Considering that the method was used on functions that have multiple roots and roots quite close to each other, the above results do not represent unacceptable numbers of false solutions. If Eq. (29) is used to calculate the relative error at a simultaneous shift for the eigenvalues for calculations of up to 20 eigenvalues, it is recommended to calculate 6 − 8 more than the actual desired number of eigenvalues. If Eq. (30) is used for calculations of up to 20 eigenvalues, it is recommended to calculate 2 − 3 more eigenvalues than the actual desired number.

Figures 4 – 8 present estimates of the calculation time required for the following conditions: a user applies Eq. (29) to find the relative error at simultaneous shift (SCG-3 in the figure), he uses Eq. (30) (SCG-4), and he uses the shifted origin inverse power law method (SCG0, only the simultaneous shifted inverse power method). These figures only show the times for the minimum eigenvalues, the greatest eigenvalues, and the intermediate eigenvalues that require the longest calculation times. SCG0 results in no false solutions and can be considered a stable collision method. When calculating a 2D problem by SCG0, however, the calculation times for 20 intermediate eigenvalues near another eigenvalue are 32 – 656 times the calculation times for 20 eigenvalues near the minimum eigenvalue. These examples show the heavy load posed in calculation of intermediate eigenvalues, which do indeed require considerably more calculation time.

The reader can see in the figures that the calculation times under the proposed procedure are less than half of those required by SCG0. However, the proposed method also misses some eigenvalues, so it is vital to select the correct values for the relative error at a simultaneous shift. SCG-3 requires less calculation time than SCG-4, but generates more false solutions; SCG-4 is slower but more stable with less false solutions. Both solvers are faster than SCG0: SCG-4 needed approximately half the time, and SCG-3 required approximately 1/5 the time needed by SCG0.

4.2 Generalized Eigenvalue Problem (2-dimensional FEM Frame Problem)

The second example problem considered is the generalized eigenvalue problem arising from the application of the finite element method (FEM) to the architectural frame with rigid nodes as shown in Fig.9. In the frame, pillars and beams are ferroconcrete, whose Young's modulus and density are 2.058×10^4N/mm^2 and 2.4×10^{-6}kg/mm^3 respectively. The cross sections (width × height) of the columns and girders are 800mm×800mm and 400mm×800mm respectively. The material length (floor height and span) are 3000mm and 6000mm respectively.

Each node of the frame has three degrees of freedom (u: displacement along x-axis, v: displacement along y-axis, θ: deflection angle), and the coefficient matrices A (stiffness matrix) and B (mass matrix) have different dimensions. Furthermore, the numerical values of the elements associated u, v and θ in the matrix A differ significantly. The matrix B was defined to be a distributed rather than concentrated mass matrix.

Table 2 shows the parameters mr, nr and n used in this experiment. Double precision arithmetic is used for all numerical calculations. The number of eigensolutions sought is

Table 2. Parameters of the frame model

model	type	mr	nr	n
B	B-1	16	14	720
	B-2	32	29	2880
	B-3	48	44	6480

mr : numbers of story, nr : numbers of span,
n : degrees of freedom

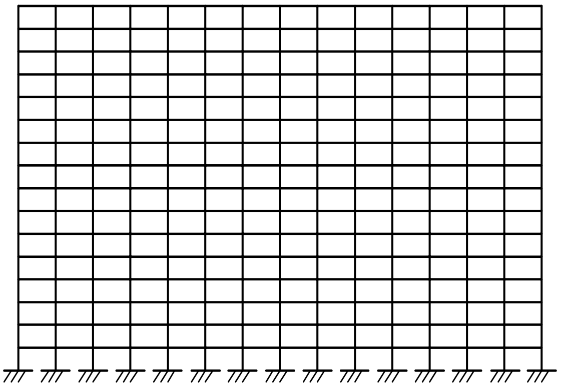

Figure 9. A plane frame model

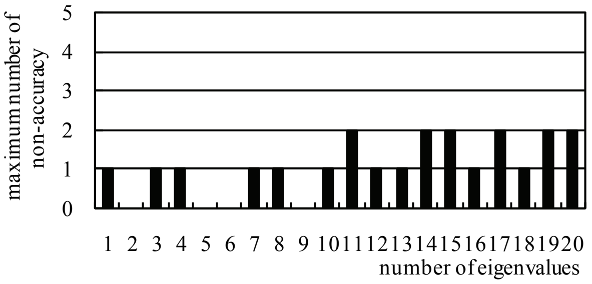

Figure 10. Maximum number of non-accuracy (frame model, Eqs.(31))

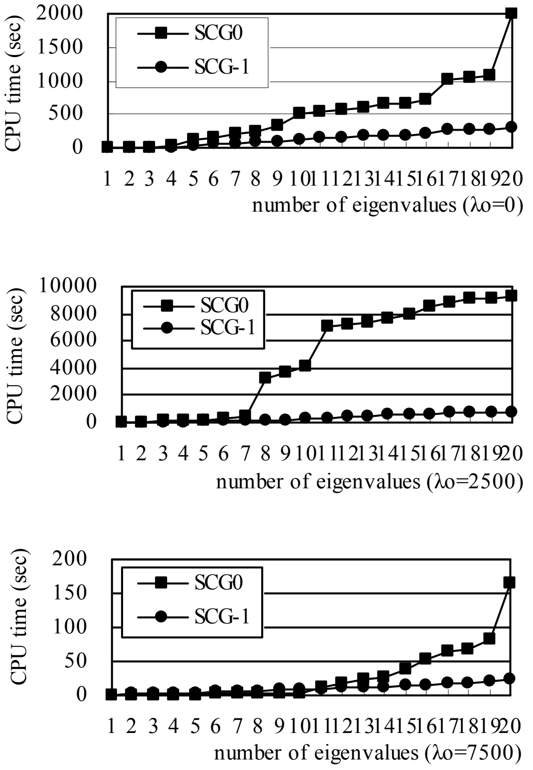

Figure 12. Computing time (frame model, type B-2)

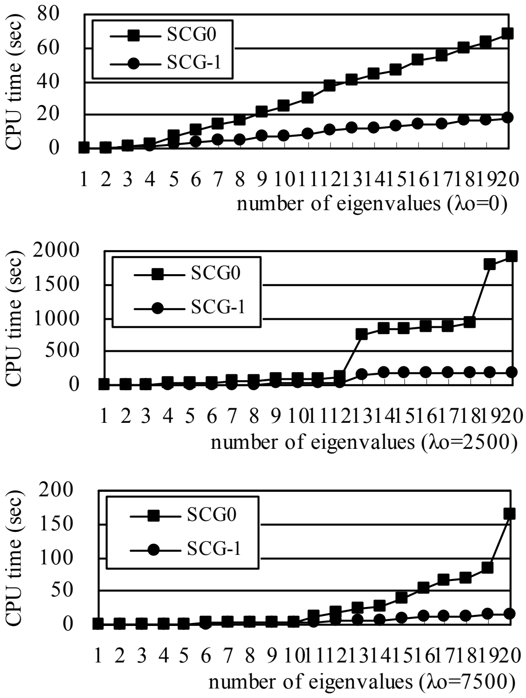

Figure 11. Computing time (frame model, type B-1)

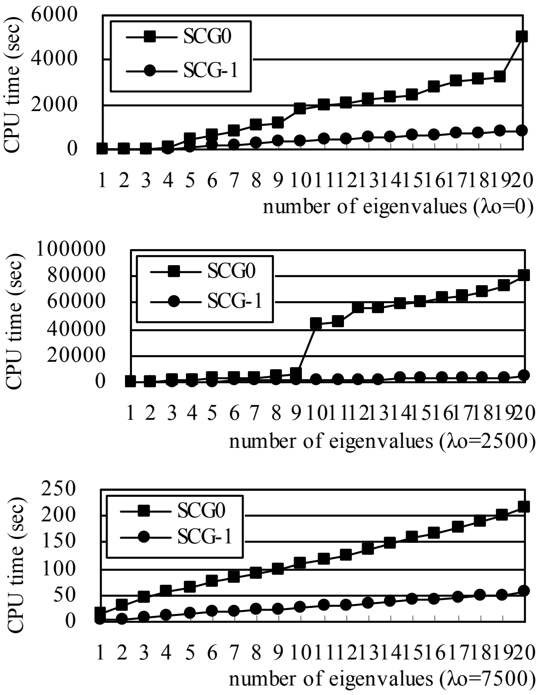

Figure 13. Computing time (frame model, type B-3)

$l = 1 \sim 20$. The initial vector is specified at random.

Although calculation of Eq. (32) needs to solve the linear equation about a mass matrix, it is computed by the diagonal matrix approximated using an element mass procession given by the following equation:

$$B = \frac{\rho A \ell}{2} \begin{bmatrix} 1 & & & & & \\ & 1 & & & 0 & \\ & & \frac{\ell^2}{210} & & & \\ & & & 1 & & \\ & 0 & & & 1 & \\ & & & & & \frac{\ell^2}{210} \end{bmatrix}$$

B : element mass matrix, ρ : density, A : cross-section area, ℓ : length of element

Figure 10 shows the maximum values of the incorrect answers in all the models. If Eq. (31) is used for calculation of the relative error at a simultaneous shift, at most two incorrect answers exist in the 2D frame model.

If Eq. (31) is used to calculate the relative error at a simultaneous shift for the eigenvalues for calculations of up to 20 eigenvalues, it is recommended to calculate 4 − 6 more than the actual desired number of eigenvalues.

Figures 11 – 13 present estimates of the calculation time required for the following conditions: a user applies Eq. (31) to find the relative error at simultaneous shift (SCG-1 in the figure), and he uses the shifted origin inverse power law method (SCG0, only the simultaneous shifted inverse power method). These figures only show the times for the minimum eigenvalues, the greatest eigenvalues, and the intermediate eigenvalues that require the longest calculation times. SCG0 results in no false solutions and can be considered a stable collision method. When calculating a 2D frame problem by SCG0, however, the calculation times for 20 intermediate eigenvalues near another eigenvalue are 4 – 53 times the calculation times for 20 eigenvalues near the minimum eigenvalue. These examples show the heavy load posed in calculation of intermediate eigenvalues, which do indeed require considerably more calculation time.

The reader can see in the figures that the calculation times under the proposed procedure are less than half of those required by SCG0. However, the proposed method also misses some eigenvalues, so it is vital to select the correct values for the relative error at a simultaneous shift.

5. SUMMARY

3D Helmholtz eigenvalue problems and plane frame problems were solved in numerical experiments using the proposed double shifted inverse power law method in an attempt to identify appropriate values for the relative error at simultaneous shift and the appropriate number of eigensolutions to be used. The following findings were made:

(1) Extremely long solution times are an issue with intermediate eigenvalues (several tens to several hundreds of times as long as those needed to find eigenvalues in the vicinity of the minimum eigenvalue). The classical shifted origin inverse power law method is a stable method that “found” no false values in this numerical experiment, but it poses a higher calculation load. The load of the proposed double shifted inverse power law method is lower, and even though it outputs some false solutions, this method proved to be stable. Programming of this method is also simple, as only a small addition to the classical shifted origin inverse power code is necessary.

(2) In the standard eigenvalue problem, the user should add at least 4 to the number of desired output eigenvalues when Eq. (29) is used to estimate the relative error at simultaneous shift to obtain up to approximately 20 correct eigenvalues. If employing Eq. (30) for the same number of desired eigenvalues, the user should add at least 1 extra. Setting the value for the relative error at simultaneous shift with Eq. (29) results in a shorter calculation time than setting it with Eq. (30), but this setting also results in more false solutions. Conversely, using Eq. (30) lengthens the calculation time but is more stable with fewer false solutions. Both equations allow shorter calculation times than the classical inverse power law method. The time is reduced by a factor of 2 if using Eq. (30), and by a factor of 5 if using Eq. (29).

(3) In the generalized eigenvalue problem, the user should add at least 2 to the number of desired output eigenvalues when Eq. (31) is used to estimate the relative error at simultaneous shift to obtain up to approximately 20 correct eigenvalues. Conversely, using Eq. (31) lengthens the calculation time but is more stable with fewer false solutions. This equation allows shorter calculation times than the classical inverse power law method.

As mentioned above, the number (m) of eigenvalues actually computed to the number (k) of desired eigenvalues is good by $m = \min\,(3k\,,\;k+8)$. It is shown from the numerical experiment which almost has neither multiple roots nor roots extremely close to each other in value that $\varepsilon_e = \min\,\left(10^{-1}/(\lambda_0+1),10^{-5}\right)$ is sufficient as the relative error of the eigenvalue at the simultaneous shift. Moreover, what is necessary is just to multiply an upper ε_e by 10^{-2}, when there are many multiple roots and roots extremely close to each other in value.

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