SHORT NOTE

Application of Preconditioned Conjugate Gradient Method to Eigenvalue Problems for One-Group Neutron Diffusion Equation

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One-group neutron diffusion theory is the most simple approximation to describe neutron behavior in the nuclear reactor, hence this approximation is often utilized for preliminary survey of reactor core design. The application of finite-difference method to the neutron diffusion equation leads to a general eigenvalue problem. In order to solve this problem, the power method is applied frequently. However, this method consists in inner iteration (solving linear systems) and outer iteration (calculation of source and eigenvalue), and the computation of eigenvalue and eigenvector becomes expensive. On the other hand, the Rayleigh quotient minimization technique by using the conjugate gradient method does not need inner-outer iterations, and has the quadratic convergence in the neighborhood of the eigensolution(1), apart from round-off errors.

In the present study we applied this method to some one-group diffusion equations. In addition to this original method, since the convergence of the algorithm depends on the condition number of coefficient matrix, we employed a preconditioner which improves the condition number of coefficient matrix. These methods were compared with the power method.

1. Rayleigh Quotient Minimization by Preconditioned Conjugate Gradient Method

The finite-difference discretization of the one-group diffusion equation leads to the matrix eigenvalue problem

$$A\phi = \lambda F\phi,$$  (1)

where $\phi$ is the scalar neutron flux vector and $\lambda$ the eigenvalue which is the inverse of the effective multiplication factor. The matrix $A$ is a positive definite matrix composed of the discretized Laplacian operator $-\nabla (D\nabla \phi)$ and neutron absorption term. The matrix $F$ is the diagonal matrix representing fission source term. The matrix $A$ is generally nonsymmetric, but becomes symmetric in rectangular geometry with equidistance meshes. Throughout this note, only cases in which $A$ is symmetric matrix will be considered.

By using the conjugate gradient method, Geradin developed a new algorithm for solving the general eigenvalue problem arising from the structural dynamic analysis(1). This method consists in seeking the stationary points of the Rayleigh quotient

$$R(\phi) = \frac{(\phi, A\phi)}{(\phi, F\phi)}$$  (2)

by minimization techniques.

This process guarantees, apart from round-off errors, the quadratic convergence in the neighborhood of the eigensolution(1). The numerical experiments have shown that the convergence of the algorithm is very sensitive to the ellipticity of $A$, which can be measured by the condition number(2). In order to improve the condition number of $A$, we utilized two preconditioners $U^T DU$ which are based on the incomplete factorization, where matrices $U^T DU$ resemble $A$. The first preconditioner is the incomplete Choleski decomposition developed by Meijerink et al.(3) and the second is the modified incomplete Choleski decomposition proposed by Gustafsson(4). The matrix $U$ is an upper triangular matrix and forced to have

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the same sparsity pattern as the upper triangular part of \( A \). The matrix \( D \) is a diagonal matrix equal to the inverse of the diagonal of \( U \). Then one can transform the Rayleigh quotient (2) in the form

\[
R(\phi) = \langle \phi, A\phi \rangle / \langle \phi, F\phi \rangle,
\]

where

\[
\widetilde{A} = (D^{1/2}U)^{-T}A(D^{1/2}U)^{-1},
\]

\[
\widetilde{F} = (D^{1/2}U)^{-T}F(D^{1/2}U)^{-1},
\]

\[
\alpha^+ = -v + \sqrt{v^2 - 4uv}/2u,
\]

\[
\alpha^- = -v - \sqrt{v^2 - 4uv}/2u,
\]

\[
\alpha_i = \max\{\alpha^+, \alpha^-\} \quad \text{for} \quad u > 0,
\]

\[
\alpha_i = \min\{\alpha^+, \alpha^-\} \quad \text{for} \quad u < 0,
\]

\[
\phi_{i+1} = \phi_i + \alpha_i s_i,
\]

\[
\lambda_{i+1} = (\phi_{i+1}, A\phi_{i+1})/(\phi_{i+1}, F\phi_{i+1}),
\]

\[
g_{i+1} = 2(A\phi_{i+1} - \lambda_{i+1} F\phi_{i+1})/(\phi_{i+1}, F\phi_{i+1}),
\]

\[
\beta_i = \frac{[\left(UT^{\top}DU\right)^{-1}g_{i+1}]^T(A - \lambda_{i+1} F)s_i - [\left(UT^{\top}DU\right)^{-1}g_{i+1}]^Tg_{i+1}(\phi_{i+1}, Fs_i)}{s_i^T(A - \lambda_{i+1} F)s_i},
\]

\[
s_{i+1} = -(UT^{\top}DU)^{-1}g_{i+1} + \beta_i s_i.
\]

2. Numerical Results

The preconditioned conjugate gradient method described in the preceding section was applied to some eigenvalue problems for one-group diffusion equation. In this study we adopted the incomplete Choleski decomposition\(^{(3)}\) and the modified incomplete Choleski decomposition\(^{(4)}\) as preconditioner (see Eqs. (4) \(\sim\) (6)).

The convergence rates were evaluated for two problems, where uniform rectangular mesh was chosen as \(\Delta x = \Delta y = 3\) cm, which resulted in 50 \(\times\) 50 mesh points.

Problem 1 is a homogeneous reactor in two-dimensional rectangular geometry. The group constants are shown in Table 1.

<table>
<thead>
<tr>
<th>Table 1 Group constants for Problem 1</th>
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<tbody>
<tr>
<td>(\Sigma_f) (cm(^{-1}))</td>
</tr>
<tr>
<td>(\Sigma_n) (cm(^{-1}))</td>
</tr>
<tr>
<td>(D) (cm)</td>
</tr>
<tr>
<td>(B^t) (cm(^{-3}))</td>
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In order to examine the effect of nonuniform configurations, we studied the second problem.

Problem 2 is an extremely heterogeneous geometry shown in Fig. 1. The group constants are the same as for Problem 1 except for \(\Sigma_n\).
All calculations were performed on the HITAC M-280H computer in double precision arithmetic.

Numerical results obtained by preconditioned conjugate gradient method are compared with power method. We employed successive over-relaxation method in the inner iteration and does not use any acceleration technique in the outer iteration. Since the convergence rate depends on the truncation number of inner iteration and the acceleration parameter of successive over-relaxation method, we performed parameter survey, then determined optimum truncation number of inner iteration and the acceleration parameter.

The convergence behavior for Problem 1 are shown in Fig. 2. The vertical axes in Fig. 2 (a), (b) denotes relative residual $\|\lambda_i F \phi_i - A \phi_i\|_2$ and relative change of eigenvalue $|\lambda_i - \lambda_{i-1}|/|\lambda_i|$, respectively, where $i$ represents the $i$-th iteration. In the case of power method (SOR), $i$ denotes the number of outer iteration. Both curves (see Fig. 2 (a), (b)) show that two preconditioned conjugate gradient methods (ICCG based on the incomplete Choleski decomposition and MICCG based on the modified incomplete Choleski decomposition) converge rapidly compared with both original conjugate gradient method (CG) and power method (SOR). The fastest convergence was obtained by MICCG method. In the case of power method, the oscillation of convergence curve for the eigenvalue is observed (see Fig. 2 (b)).

The convergence behavior for Problem 2 are shown in Fig. 3. The conjugate gradient method (CG) and power method (SOR) show slow convergence compared with Problem 1. On the other hand, ICCG and MICCG methods converge still rapidly in the same way as Problem 1.

The computational time for Problem 2 to achieve the relative residual $\leq 10^{-7}$ are shown in Table 2. It is remarkable that MICCG method is very fast compared to the other methods.
3. Conclusions

The Rayleigh quotient minimization using preconditioned conjugate gradient method showed very fast convergence compared with original conjugate gradient method and power method using successive over-relaxation method in the inner iteration, and reduced computational time. Especially preconditioned conjugate gradient method with modified incomplete Choleski decomposition was effective for both of the convergence rate and computational time.

REFERENCES

(2) idem : ibid., 19, 111 ~ 132 (1971).
(4) GUSTAFSSON, I. : BIT, 18, 142 ~ 156 (1978).