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RQI 기법의 성능 개선

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Improvement of the Rayleigh Quotient Iteration Method

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Abstract-When a few eigenvalues and eigenvectors are desired, Rayleigh Quotient Iteration(RQI) is widely used. The RQI, however, cannot give maximum or minimum eigenvalue/eigenvector. In this paper, Modified Rayleigh Quotient Iteration(MRQI) is developed. The MRQI can give the maximum or minimum eigenvalue/eigenvector regardless of the initial starting vector.

1. Introduction

The RQI[1,2], developed by Lord Rayleigh, is a powerful tool in dealing with the symmetric eigenvalue problem. When maximum or minimum eigenvalue and the corresponding eigenvector are desired, the RQI, however, cannot give them for arbitrary initial starting vector. This phenomenon result from the local convergence property of RQI that is found by Ostrowski. For Hermitian matrices, Ostrowski describes a finite neighborhood(unknown a priori) around each eigenvector. When the RQI is started in this region, convergence will occur to the associated eigenvector[3]. Consequently, if the initial starting vector is not determined properly, the classical RQI can give neither maximum nor minimum eigenvalue and the corresponding eigenvector.

2. Derivation of the MRQI

In this paper, the MRQI is developed which can give maximum/minimum eigenvalue and the associated eigenvector regardless of the initial starting vector. The following algorithm represents the MRQI. Suppose $A \in \Re^{n \times n}$ is symmetric and z is a given non-zero n-vector. Assume that the arbitrary initial starting vector z_0, such that $\|z_0\|_2 = 1$, is given.

Step 1. Form the Rayleigh Quotient of z_k

$$\mu(z_k) = \frac{z_k^T A z_k}{z_k^T z_k}.$$

Step 2. Calculate the α_k and solve $(A - \alpha_k \mu_k I) v_{k+1} = z_k$ for v_{k+1}.

Step 3. Normalize $z_{k+1} = v_{k+1} / \gamma_{k+1} \quad (\gamma_{k+1} = \|v_{k+1}\|_2)$

Step 4. Check the stopping criterion. If the criterion is not satisfied, return the Step 1 until the criterion is satisfied.

The key idea of MRQI lies in adding a new variable α_k in Step 2. The global convergence and detailed analysis of MRQI will be described in subsequent paper, since they require much space. The following theorem says that the

MRQI can give the maximum/minimum eigenvalue and the corresponding eigenvector with a proper selection of α_k regardless of the starting initial vector.

Theorem 1 Let $A \in \Re^{n\times n}$ be a given symmetric positive definite matrix. Assume that the MRQI converges to a eigenvalue and the corresponding eigenvector. For an arbitrary initial starting vector, the following results then hold.

i) If $\alpha_k \geq \frac{\|A\|_\infty}{\mu_k}$, then the MRQI converges to the maximum eigenvalue and the corresponding eigenvector.

ii) If $\alpha_k \leq 0$, then the MRQI converges to the minimum eigenvalue and the corresponding eigenvector.

proof) Since global convergence to any eigenvalue and the corresponding eigenvector is assumed, it is sufficient to prove that the converged eigenvalue/eigenvector corresponds to maximum or minimum eigenvalue/eigenvector with given α_k, respectively. Assume that A has a basis of eigenvectors $\{x_1,\cdots,x_n\}$ and that $Ax_i=\lambda_i x_i$ for $i=1,2,\cdots,n$.

i) Assume that $\lambda_1>\lambda_2\geq\cdots\geq\lambda_n$. If $z_0=\sum_{i=1}^{n}\beta_i x_i$, then

$$\prod_{i=k}^{0}(A-\alpha_i\mu_i)^{-1}z_0=\prod_{i=0}^{k}\frac{\beta_1}{(\lambda_1-\alpha_i\mu_i)}(x_1+\frac{\beta_2}{\beta_1}\prod_{i=0}^{k}\frac{(\lambda_1-\alpha_i\mu_i)}{(\lambda_2-\alpha_i\mu_i)}x_2$$

$$+\cdots+\frac{\beta_n}{\beta_1}\prod_{i=0}^{k}\frac{(\lambda_1-\alpha_i\mu_i)}{(\lambda_n-\alpha_i\mu_i)}x_n)$$

where

$$\prod_{i=a}^{i=b}A_i\equiv A_aA_{a-1}\cdots A_b \text{ for all integer } a,\ b.$$

It follows that if we define

$$q_{k+1}=\frac{z_{k+1}}{\gamma_1\gamma_2\cdots\gamma_k}\prod_{i=0}^{k}(\lambda_1-\alpha_i\mu_i),$$

then

$$q_{k+1}=\beta_1x_1+\prod_{i=0}^{k}\frac{(\lambda_1-\alpha_i\mu_i)}{(\lambda_2-\alpha_i\mu_i)}\beta_2x_2+\cdots+\prod_{i=0}^{k}\frac{(\lambda_1-\alpha_i\mu_i)}{(\lambda_n-\alpha_i\mu_i)}\beta_nx_n$$

If $\alpha_k\geq\frac{\|A\|_\infty}{\mu_k}$, then $\left|\frac{\lambda_1-\alpha_i\mu_i}{\lambda_j-\alpha_i\mu_i}\right|<1$ for all $i=1,2,\cdots,k$ and $j=2,3,\cdots,n$ by the assumption $\lambda_1>\lambda_2\geq\cdots\geq\lambda_n$ and Gershigorin's circle theorem. Therefore

$$\lim_{k=\infty}\prod_{i=0}^{k}\frac{\lambda_1-\alpha_i\mu_i}{\lambda_j-\alpha_i\mu_i}=0 \text{ for all } i=1,2,\cdots,k \text{ and } j=2,3,\cdots,n.$$

Hence if $\beta_1\neq 0$,

$$\lim_{k=\infty}q_{k+1}=\beta_1x_1.$$

Thus the sequence $\{q_i,\ i=1,2,\cdots\}$(that is $\{z_i,\ i=1,2,\cdots\}$) approximates the eigenvector associated with maximum eigenvalue with increasing accuracy.

ii) In this case, if we assume that $\lambda_1\geq\cdots\geq\lambda_{n-1}>\lambda_n$ and that $\beta_n\neq 0$, then the assertion is proved by similar procedure. ■

In the case of RQI, when RQI is started in the neighborhood of a eigenvector, the sequence $\{z_i,\ i=1,2,\cdots\}$ cannot go out the neighborhood and must converge to the eigenvector. Therefore the RQI has not been able to give a convergence to maximum or minimum eigenvalue and the corresponding eigenvector. However the new added variable α_k in MRQI enables the sequence $\{z_i,\ i=1,2,\cdots\}$ to move from the neighborhood of a eigenvector to the neighborhood of another eigenvector. The above theorem means that a proper selection of α_k have the sequence $\{z_i,\ i=1,2,\cdots\}$ move inside of the neighborhood of the eigenvector associated with the maximum or minimum eigenvalue.

The condition $\beta_1\neq 0$ or $\beta_n\neq 0$ is not a severe restriction. This condition will usually be satisfied by almost any randomly chosen initial vector z_0.

In the MRQI, if the variable α_k is selected as constant, then the convergence rate may be slow down depending on the initial starting vector. In this case, α_k can be determined as exponential function of k, i. e., $\alpha_k=a+be^{(-k/c)}$, to speed up the convergence rate.

3. A Numerical Example

The following example shows that the MRQI can give maximum/minimum eigenpair.

Example 1[[1], p.309] The matrix

$$A=\begin{bmatrix}1&1&1&1&1&1\\1&2&3&4&5&6\\1&3&6&10&15&21\\1&4&10&20&35&56\\1&5&15&35&70&126\\1&6&21&56&126&252\end{bmatrix}$$

has eigenvalues {0.0030, 0.0643, 0.4893, 2.0436, 15.5535, 332.8463}. The MRQI is applied to the matrix with $z_0=(1,1,1,1,1,1)^T/\sqrt{6}$, then the following results are obtained.

Table 1.$(a=1.0,\ b=\|A\|_\infty,\ c=6.0)$

iteration k	μ_k
0	153.8333
1	332.8145
2	332.8463
3	332.8463
4	332.8463

Table 2.$(a=1.0,\ b=-1.01,\ c=0.01)$

iteration k	μ_k
0	153.8333
1	0.9645
2	0.0387
3	0.0031
4	0.0030
5	0.0030
6	0.0030

The iteration is converging to the maximum(Table 1)/minimum(Table 2) eigenvalue. ■

4. Conclusion

In this paper, the MRQI, which can give maximum/minimum eigenpair, is developed. The MRQI is regard as generalized iteration in that if $\alpha_k=1$, the MRQI becomes the normal RQI, if $\alpha_k=0$, the MRQI becomes the inverse power method, and if $\alpha_k=\hat{\lambda}/\mu_k$ ($\hat{\lambda}$ is an estimate of an eigenvalue), the MRQI becomes inverse iteration(shifted inverse power method).

Reference

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