Test Method for a Computer Program of Characteristic Equations

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Abstract

At the present time, there are many library programs for characteristic equations. But, owing to the variety of the programs, a programmer is often unable to determine which program is the most appropriate for his aim. Unfortunately, there are few powerful methods to test the reliability of the library programs[1]. Actually, some textbooks[2,3] show only test matrices. In this paper, we show a test method for the reliability of the library programs for characteristic equations of real symmetric matrices. The test can be carried out without the detailed knowledge about the algorithm of the tested program.

1. Introduction :

The test method for characteristic equations is formulated to fulfil the following two requirements with a similar motivation to that of ref[4].

(1) The results of the test can be estimated under a certain mathematical criterion.

(2) The test is systematically executed in a simple mechanical technic.

In order to fulfil the requirements, the numerical solutions are analyzed with some mathematical properties of eigenvalues and eigenvectors. The results of these analyses give us a certain standard to estimate the errors of numerical solutions. Furthermore, in our test method, the test matrices can be generated with known eigenvalues and eigenvectors in an arbitrary condition(for example, the test matrix has a very large and a very small eigenvalue). Then, we can test a program under an arbitrary condition. The test matrix A is not necessarily large dimensional. Then, the test can be economically executed with the use of 3×3 dimensional matrices.

2. Characteristic Equation and its Approximate Solution :

Let A be an $n\times n$ matrix with eigenvalues λ_i and eigenvectors $\vec{x}_i$, $i=1,2,\ldots,n$:

$$A\vec{x}_i = \lambda_i\vec{x}_i \ . \tag{2.1}$$

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An approximate solution $(\lambda_i', \vec{x}_i')$ of Eq.(2.1) can be expanded with the exact solutions,

$$\vec{x}_i' = (1 - \delta_i)\vec{x}_i + \delta_\perp \sum_{j\neq i} \alpha_{ij}\vec{x}_j, \quad \lambda_i' = \lambda_i + \delta\lambda_i. \qquad (2.2)$$

The error vector $\delta\vec{x}_i'$ is expressed by the form : $\delta\vec{x}_i = \vec{x}_i' - \vec{x}_i$. Here, δ_i is the component of $\delta\vec{x}_i'$ parallel to $\vec{x}_i$, and $\delta_\perp$ is that perpendicular to the $\vec{x}_i$. $\delta\lambda_i$ is the error for λ_i'. $\delta_\perp$ and δ_i are determined with the orthonormalization of eigenvectors. The inner-product between $\vec{x}_i'$ and $\vec{x}_j$ in Eq.(2.2) yields : $\delta_\perp \alpha_{ij} = \langle \vec{x}_i' \cdot \vec{x}_j \rangle$, $i\neq j$. On the assumption $|\sum_{j\neq i} \alpha_{ij}\vec{x}_j| = 1$, α_{ij} satisfy the relation : $\sum_{j\neq i} \alpha_{ij}^2 = 1$. So that, we can obtain the following expressions,

$$\delta_\perp = \sqrt{\delta_\perp^2 \sum_{j\neq i} \alpha_{ij}^2} = \sqrt{\sum_{j\neq i} \langle \vec{x}_j \cdot \vec{x}_i' \rangle^2}, \qquad (2.3)$$

$$\delta_i = 1 - \langle \vec{x}_i \cdot \vec{x}_i' \rangle, \qquad (2.4)$$

$$\alpha_{ij} = \langle \vec{x}_j \cdot \vec{x}_i' \rangle / \delta_\perp, \quad j\neq i. \qquad (2.5)$$

Any real floating-point numbers generally have the relative error Δ which depends on an individual computer. An approximate solution $(\lambda_i', \vec{x}_i')$ is expected to be solved within the error Δ. Thus, the angle Ω between the vectors $A\vec{x}_i'$ and $\lambda_i'\vec{x}_i'$ should be approximately equal to zero within the error Δ.

$$0 \leqq |1-\cos\Omega| \leqq |1-\cos\Delta|, \qquad (2.6)$$

where

$$\cos\Omega = \frac{\lambda_j'}{|\lambda_j'|} \cdot \frac{(1-\delta_i)^2\lambda_i + \delta_\perp^2 \sum_{j\neq i} \alpha_{ij}^2 \lambda_j}{\sqrt{[(1-\delta_i)^2 + \delta_\perp^2] \cdot [(1-\delta_i)^2\lambda_i^2 + \delta_\perp^2 \sum_{j\neq i} \alpha_{ij}^2 \lambda_j^2]}}$$

The difference between the lengths $\|A\vec{x}_i'\|$ and $\|\lambda_i'\vec{x}_i'\|$ of the vectors $A\vec{x}_i'$ and $\lambda_i'\vec{x}_i'$ should satisfy the following relation : $f \equiv |\|A\vec{x}_i'\| - \|\lambda_i'\vec{x}_i'\|| / |\lambda_{max}| \leqq \Delta$, (2.7)
Here, $A\vec{x}_i' = \sqrt{(1-\delta_i)^2\lambda_i^2 + \delta_\perp^2 \sum_{j\neq i} \alpha_{ij}^2 \lambda_j^2}$ and $\lambda_i'\vec{x}_i' = \sqrt{\lambda_i'^2[(1-\delta_i)^2 + \delta_\perp^2]}$.

The value of $|\delta\vec{x}_i|$ depends on A. If λ_i and λ_j are multiple eigenvalues, orthogonality of $\vec{x}_i$ and $\vec{x}_j$ can not uniquely determined. This is one of the causes for the error vector $\delta\vec{x}_i$. For example, when λ_i' approaches to λ_j', it becomes difficult to determine the orthogonality between the vectors $\vec{x}_i'$ and $\vec{x}_j'$. Then, $\vec{x}_i'$ may have much component of $\vec{x}_j$. This means that $|\delta\vec{x}_i|$ becomes large. Thus, the value of $|\delta\vec{x}_i|$ may vary as the $(\lambda_i, \vec{x}_i)$ varies. And also, δ_i, $\delta_\perp\alpha_{ij}$ and $\delta\lambda_i$ have the same causes as $\delta\vec{x}_i$. On the contrary, f and $|1-\cos\Omega|$ should be suppressed by the upper boundaries Δ and $|1-\cos\Delta|$. Therefore, it is reasonable to observe the systematical dependence of $\delta_\perp$, δ_i, $|\delta\vec{x}_i|$ and $\delta\lambda_i$ on $(\lambda_i,\vec{x}_i)$, and the independence of f and $|1-\cos\Omega|$ from $(\lambda_i,\vec{x}_i)$. If the results of the test do not satisfy these conditions, we should suspect the reliability of the tested program.

3. Test Matrices:

The test is systematically executed in a mechanical method. Then, the test matrices A need to be easily generated with well-known eigenvalues and eigenvectors. In concentrating our attention on an eigenvalue λ_i, we understand that λ_i surely satisfies one of the four cases: (1) the smallest, (2) neither the smallest nor the largest, (3) the largest or (4) degenerate with another eigenvalue. All of the four cases can be realized in three dimensional space. So that it is enough to use three dimensional matrices for the test about eigenvalue dependence. On the one hand, the eigenvectors need to satisfy only the orthonormal relation. Thus the test can be satisfactorily discussed in three dimensional space for eigenvectors too. Then, we discuss the test with the three dimensional matrices Λ and X.

Now, Eq.(2.1) can be rewritten in a product form of matrices: $AX=X\Lambda$. In three dimensional space, the matrices Λ and X are given as,

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \qquad (3.1)$$

$$X = (\vec{x}_1,\vec{x}_2,\vec{x}_3) = \begin{pmatrix} \cos\theta\cos\phi\cos\psi-\sin\phi\sin\psi & \cos\theta\sin\phi\cos\psi+\cos\phi\sin\psi & -\sin\theta\cos\psi \\ -\cos\theta\cos\phi\sin\psi-\sin\phi\cos\psi & -\cos\theta\sin\phi\sin\psi+\cos\phi\cos\psi & \sin\theta\sin\psi \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{pmatrix} \qquad (3.2)$$

where (ϕ,θ,ψ) are Euler angles of a rotation matrix[5]. Thus A can be generated with Λ and X: $A=X\Lambda X^T$. (3.3)

By controlling the parameters ϕ, θ, ψ, λ_1, λ_2 and λ_3 in Eq.(3.3), we can construct mechanically any test matrices. For observation of the relative error of an eigenvalue and an eigenvector, it is enough to notice the relative magnitudes of eigenvalues. Then, if λ_2 and λ_3 are fixed as constant parameters, the error of $(\lambda_1,\vec{x}_1)$ is analyzed for the variables λ_1 and (ϕ,θ,ψ). The results of the test can be plotted against λ_1 and (ϕ,θ,ψ) in cylindrical coordinates. λ_1 and (ϕ,θ,ψ) are plotted on the plane perpendicular to Z-axis. (ϕ,θ,ψ) are varied from the initial to the final point in three dimensional space under an appropriate condition. The trace of the angles is plotted in the surrounging of Z-axis. For example, if ϕ and ψ are fixed, θ is plotted around Z-axis. $|\delta\vec{x}_1|$, $\delta\lambda_1$, δ_1, $\delta_\perp$, α_{ij}, f and $\sqrt{(1-\cos\Omega)}$ are plotted along Z-axis.

4. Test Procedure and Example :

For simplicity, we show an example to test a program about λ_1. The test procedure is shown in Fig.1. In this test, we assume that $(\phi,\theta,\psi)=(45°,20°,45°)$, $\lambda_2=1.1$ and $\lambda_3=0.9$ are fixed. The eigenvalue λ_1 moves from λ_{min} to λ_{max} by the step $\Delta\lambda$. Fig.2 shows $|\delta\vec{x}_1|$ $\delta_\perp$ and $\sqrt{(1-\cos\Omega)}$ against λ_1. Fig.3 shows $\delta\lambda_1$, f and δ_1 against λ_1. For convenience, λ_1 is plotted with a logarithmic scale in areas $\lambda_1 \geqq 10$ and $\lambda_1 \leqq 0.1$, and with a linear scale in an area $0.8 \leqq \lambda_1 \leqq 1.2$. There are two blank areas at $0.845 \leqq \lambda_1 \leqq 0.950$ and $1.045 \leqq \lambda_1 \leqq 1.555$, in which the tested program cannot solve the given equations because of multiple eigenvalues of A.

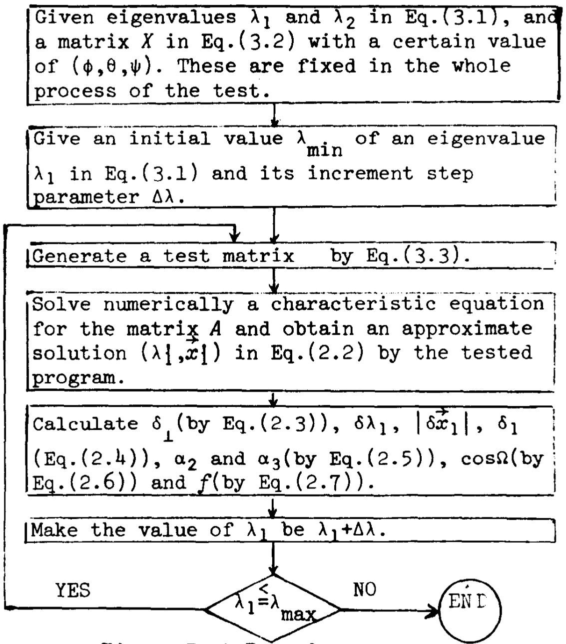

Fig.1 Test Procedure

The results of the test predict several properties of the program. The test is executed with a computer in which a real floating-point number has relative error 10^{-10}. $|\delta\vec{x}_1|$ and $\delta_\perp$ are very large for small values of λ_1 and for nearly multiple-eigenvalue state. $\sqrt{(1-\cos\Omega)}$ are expected to be constant independently of λ_1. But $\sqrt{(1-\cos\Omega)}$ in Fig.2 strongly depend on λ_1. $\sqrt{(1-\cos\Omega)}$ are nearly constant for the test of another program. Why do $\sqrt{(1-\cos\Omega)}$ strongly depend on λ_1 in this test? We feel something questionable in the tested program. In Fig.3, $|\delta\lambda_1|$ and f get very large for small value of λ_1.

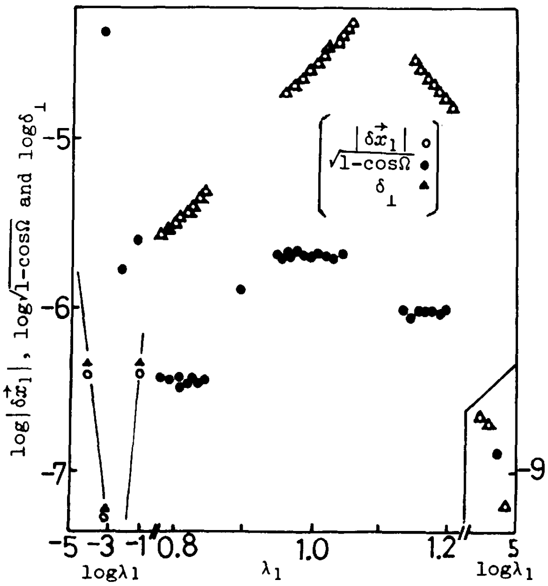

Fig.2 Results of the test for $|\delta\vec{x}_1|$, $\sqrt{1-\cos\Omega}$ and $\delta_\perp$.

The trend of $|\delta\lambda_1|$ and f in Fig.3 has a common cause of $|\delta\vec{x}_1|$ and $\sqrt{(1-\cos\Omega)}$ in Fig.2. Near multiple-eigenvalue state, f does not strongly depend on λ_1.

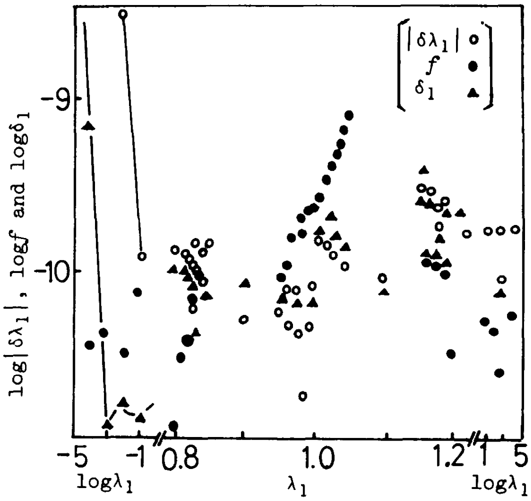

Fig.3 Results of thetest for $|\delta\lambda_1|$, f and δ_1.

5. Conclusion:

Some programmers who make use of library programs often want to know general property of these programs. By the aid of this test method, a programmer can test the programs with only those specifications without the knowledge of those detailed algorithms. If the programmer specifies only a test condition, he can estimate the reliability of the program under the condition as shown in Fig.2 and Fig.3.

Some algorithms give a part of eigenvalues and eigenvectors(for example, the largest eigenvalue). Fortunately, the test method uses only one set of an eigenvalue and an eigenvector. Thus, it is possible to execute the test for such a characteristic algorithm. In this paper, the relation between the errors and the mathematical properties of A are discussed. But the problem about an accumulation of round-off errors is left to be opened.

References

1) Cody, W. J. : Program Test Method, edited by William C. Hetzel, Prentice Hall, Inc., Engelwood, New Jersey, p121, (1972).

2) Fuller, L. E. : Basic Matrix Theory, Prentice Hall, Inc., Engelwood Cliffs, New Jersey, (1962).

3) Gear, C. W. : Math. Comp. 23, pp119-125, (1969). Gregory, R T. and D L. Karney: A Collection of Matrices for Testing Computational Algorithms, Wiley-Inc., New York, (1969).

4) Isomoto, Y. and K. Morita : Information Processing in Japan, Vol. 13, Information Processing Society of Japan, pp.19-22, (1973).

5) Brink, D M. and G. R Satchler : Angular momentum, Oxford Univ. Press, New York.