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Inverse Iteration Method with a Complex Parameter II

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§1. Introduction

Let A be a symmetric (n, n) matrix and let $\lambda_k, \phi_k, k = 1, \ldots, n$ be pairs of eigenvalues and the corresponding eigenvectors of A. The inverse iterarion process for the eigenvector ϕ_j is to solve the following linear equations with initial data $z^{(0)}$ under the conditions $|\lambda_j - \lambda| << c < |\lambda_k - \lambda|, (k \neq j)$:

$$(1.1) \qquad (A - \lambda I)z^{(m+1)} = z^{(m)}, m = 0, 1, 2, \ldots$$

In the paper [1] we proposed the inverse iteration method with a complex parameter and showed some numerical results of our method. There we replaced λ in (1.1) by a complex parameter $\lambda + \sqrt{-1}\tau$ and managed to derive the utilities of the complex parameter with $|\tau| < \varepsilon$ under the following Assumption H.

Assumption H. Eigenvalues $\lambda_k, k = 1, 2, \ldots, n$ of A are known with the following accuracy: There are three numerical constants c,ε and λ such that $\inf_{k \neq j} |\lambda_j - \lambda_k| > 2c$ and $|\lambda_j - \lambda| < \varepsilon$ and $0 < 2\varepsilon < c$.

In the spectral theory, it is well known that the projection operator P_j to the eigenspace correspondong to the eigenvalue λ_j is represented as follows

$$(1.2) \qquad P_j v = \frac{1}{2\pi\sqrt{-1}} \oint (A - \zeta I)^{-1} v d\zeta.$$

It can be considered that to solve the linear equation (1.1) is to execute the numerical integral of (1.2) with one point value. Since the result of our method is understood to be that with two point values, it will be taken for granted that our method is more effective than the standard traditional one.

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In this paper we show supplementary propositions to [1] and propose the more powerful version of our method in practical computations.

§2. Propositions and the iteration process

In the paper [1], we did not give the proofs of the propositions. The most important one of them can be improved as the following two propositions.

Consider the following equation with $\|z\| = 1$:

$$(A - \lambda I - \sqrt{-1}\tau I)w = z. \tag{2.1}$$

Let $z = \sum_{k=1}^{n} a_k \phi_k$, then we have

$$\begin{aligned} w &= \sum_{k=1}^{n} \frac{1}{\lambda_k - \lambda - \sqrt{-1}\tau} a_k \phi_k \\ &= \sum_{k=1}^{n} \frac{\lambda_k - \lambda}{(\lambda_k - \lambda)^2 + \tau^2} a_k \phi_k + \sqrt{-1} \sum_{k=1}^{n} \frac{\tau}{(\lambda_k - \lambda)^2 + \tau^2} a_k \phi_k. \end{aligned} \tag{2.2}$$

Put $x_k = \dfrac{\lambda_k - \lambda}{(\lambda_k - \lambda)^2 + \tau^2} a_k \phi_k$ and $y_k = \dfrac{\tau}{(\lambda_k - \lambda)^2 + \tau^2} a_k \phi_k$. Let $x = \sum_{k=1}^{n} x_k$ and $y = \sum_{k=1}^{n} y_k$.

Proposition 2.1. *Let x,y be the real and imaginary part of the solution of the equation (2.1) with $|\lambda_j - \lambda| < |\tau| \le \varepsilon$ under the Assumption* H *in which the inequality $|\lambda_j - \lambda| < |\varepsilon|$ is assumed. Put $\tilde{\lambda} = (Ay, y)/\|y\|^2$. If $3\|y\| > 2\|x\|$, then $|\lambda_j - \tilde{\lambda}| < |\tau|$.*

Proof. Put $\alpha_k = [(\lambda_k - \lambda)^2 + \tau^2]^{-1}$ and $T = \sum_{k=1}^{n} \alpha_k^2 a_k^2$. Since $4\varepsilon < 2c < \inf_{k \ne j} |\lambda_j - \lambda_k|$ by the assumption H. We have the following inequalities:

$$\sum_{k \ne j} |\lambda_k - \lambda|^2 \alpha_k^2 a_k^2 \ge 3\varepsilon \sum_{k \ne j} |\lambda_k - \lambda| \alpha_k^2 a_k^2$$

and

$$\sum_{k \ne j} |\lambda_k - \lambda|^2 \alpha_k^2 a_k^2 \ge 9\varepsilon^2 \sum_{k \ne j} \alpha_k^2 a_k^2.$$

Then from the assumption $3\|y\| \ge 2\|x\|$, we have

$$9\tau^2 T \ge 4 \sum_{k=1}^{n} |\lambda_k - \lambda|^2 \alpha_k^2 a_k^2 \ge 4 \cdot 3\varepsilon \sum_{k \ne j} |\lambda_k - \lambda| \alpha_k^2 a_k^2,$$

that is,

$$(2.3) \qquad \frac{3}{4}\frac{\tau^2}{\varepsilon}T \geq \sum_{k\neq j} |\lambda_k - \lambda|\alpha_k^2 a_k^2.$$

Similarly we also have the following inequality:

$$(2.4) \qquad \frac{1}{4}\frac{\tau^2}{\varepsilon^2}T \geq \sum_{k\neq j} \alpha_k^2 a_k^2.$$

On the other hand, we have following estimates:

$$\begin{aligned}|\lambda_j - \tilde{\lambda}| &= |\lambda_j - (Ay, y)/\|y\|^2| \\ &= |\lambda_j - (\sum_{k=1}^{n} \lambda_k \tau^2 \alpha_k^2 a_k^2 / \sum_{k=1}^{n} \tau^2 \alpha_k^2 a_k^2)| \\ &\leq \sum_{k\neq j} |\lambda_j - \lambda_k|\alpha_k^2 a_k^2/T \\ &\leq \sum_{k\neq j} |\lambda_j - \lambda|\alpha_k^2 a_k^2/T + \sum_{k\neq j} |\lambda - \lambda_k|\alpha_k^2 a_k^2/T.\end{aligned}$$

So we have the following results from (2.3) and (2.4):

$$|\lambda - \tilde{\lambda}| \leq |\tau|\frac{1}{4}\frac{\tau^2}{\varepsilon^2} + \frac{3}{4}\frac{\tau^2}{\varepsilon} \leq |\tau|.$$

Q.E.D.

The following proposition is easily derived by a similar argument used in the proof of the Proposition 2.1.

Proposition 2.2. *Under the same assumption of Proposition* 2.1, *if* $\|y\| \geq \|x\|$ *then* $|\lambda_j - \tilde{\lambda}| < \frac{\tau^2}{c}$.

These propositions bring the following more powerful version of the iteration process of our method in [1], where the step (2.7) and (2.8) are varied.

Let ξ be an initial vector and let $\tau^{(0)}$ be a real number whose absolute value is smaller than ε. Our iteration process consists of the following four steps (2.5)–(2.8), where $u^{(m)}$ and $v^{(m)}$ are real vectors.

$$(2.5) \quad (A - \lambda^{(m)}I - \sqrt{-1}\tau^{(m)}I)w^{(m)} = z^{(m)} \qquad \text{where } z^{(0)} = \xi, \lambda^{(0)} = \lambda$$

$$z^{(m+1)} = \frac{v^{(m)}}{\|v^{(m)}\|} \quad \text{where } w^{(m)} = u^{(m)} + \sqrt{-1}v^{(m)} \tag{2.6}$$

$$\lambda^{(m+1)} = \begin{cases} (Az^{(m+1)}, z^{(m+1)}) & \text{if } 3\|v^{(m)}\| > 2\|u^{(m)}\| \\ \lambda^{(m)} & \text{otherwise.} \end{cases} \tag{2.7}$$

$$\tau^{(m+1)} = \frac{(\tau^{(m)})^2}{c} \quad \text{if } \|v^{(m)}\| > \|u^{(m)}\|. \tag{2.8}$$

Remark 2.3. The process (2.8) may be passed if $|\tau^{(m)}|$ is small enough.

§3. Applications

Propositions 2.1 and 2.2 show that even if we do not have a so accurate value of ε or even if the initial vector is not so well, $\lambda^{(m)}$ in the iteration process converges to the aimed eigenvalue efficiently by using better parameters in each iteration. So we can have an application of our method to get a rapid tool for computing eigen-pairs combining the bisection method. Its idea is such that: get rough estimates of eigenvalues by the bisection method, first, then, apply our iteration process. The computing time to improve the accuracy of an eigenvalue by 5 decimal digits with the aid of the bisection method is comparable to that of two times iterations of our method. So, for example, if, starting from the initial approximating value with the accuracy about 10^{-4}, we could have the eigenvalue with the accuracy 10^{-15} after two times iterations, this method is an improvement of the procedure done by only the bisection method. The test computations of this example and of the others of this kinds have shown satisfactory results. We do not have the optimal result as yet but the above example is at least one of the application of our method to get eigen-pairs more rapidly.

References

[1] Suzuki, T., Inverse iteration method with a complex parameter, Proc. Japan Acad. Ser. A, **68** No.3 (1992), 68–73.

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