ON CALCULATING EIGENVALUES BY THE GRADIENT METHOD

By

Seiiti HUZINO

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Let A and B be $n \times n$ matrices in an n -dimensional complex vector space V^n , and B be non-singular.

Consider the eigenvalue problem

$$(1) \quad Ax = \lambda Bx,$$

where λ is a complex parameter. When $x \neq 0$ satisfies (1) for a value λ of the parameter, we call the point $y = (x^1, x^2, \dots, x^n, \lambda)$ in the space $V^n \times C$ the eigenpoint, C being the space of complex numbers.

Let H be a prescribed positive definite Hermitian matrix and define an error function

$$(2) \quad E(y) = E_\lambda(x) = (Ax - \lambda Bx, H(Ax - \lambda Bx))_{V^n},$$

where the bracket means the scalar product in the space V^n . y is an eigenpoint in $V^n \times C$ if and only if $x \neq 0$ and $E(y) = 0$.

Let us put

$$(3) \quad L = A^*HA, \quad M = B^*HA, \quad N = B^*HB,$$

then L is a positive semi-definite Hermitian matrix, and N is a positive definite Hermitian matrix.

Furthermore, we consider the following non-linear transformation μ from $V^n \ominus \{0\}$ into C :

$$(4) \quad \mu(x) = (Mx, x) / (x, Nx).$$

If $x \neq 0$ is an eigenvector corresponding to an eigenvalue λ , then

$$(5) \quad \mu(x) = \lambda.$$

In general it holds

$$(6) \quad E_{\lambda}(x) = (x, Nx)|\lambda - \mu(x)|^2 + (x, Lx) - |\mu(x)|^2(x, Nx),$$

and we have the relation

$$(7) \quad E_{\mu(x)}(x) = (x, Lx) - |\mu(x)|^2(x, Nx)$$

for the point $y = (x, \mu(x))$. When x is an eigenvector, $\mu(x)$ being its corresponding eigenvalue, we obtain from (6)

$$(8) \quad E_{\lambda}(x) = (x, Nx)|\lambda - \mu(x)|^2$$

and

$$(9) \quad E_{\mu(x)}(x) = 0.$$

The formula (6) shows the fact that for each fixed value of x , $E_{\lambda}(x)$ takes the minimum value (7) when $\lambda = \mu(x)$, especially the value 0 for an eigenvector x .

Our object is to derive a suitable numerical method of determining the eigenpoints y by using the above facts. We shall at first restrict ourselves to the case when all eigenvalues are real. For instance the case when A is real symmetric, H is positive symmetric and B is the identity matrix belongs to the case. Another example is the case when A^*H and B^*H are both Hermitian. Using an analogous algorithm used in the Hestenes' conjugate gradient method ([1]) for solving linear systems, we consider the following algorithm:

(a) We select a suitable positive Hermitian (or real symmetric) matrix K . We put $A = N^*HN$. Then A is a positive definite Hermitian matrix.

(b) For the points x_i and $p_{i,0}$ ($i=0, 1, 2, \dots$), we seek the following points:

$$(10) \quad r_{i,0} = M^*x_i - \mu(x_i)Nx_i - Np_{i,0},$$

$$(11) \quad g_{i,0} = N^*Hr_{i,0} \quad (= N^*HM^*x_i - \mu(x_i)Ax_i - Ap_{i,0}),$$

$$(12) \quad q_{i,0} = Kg_{i,0}.$$

(c) For the points $p_{i,j}$, $r_{i,j}$, $g_{i,j}$ and $q_{i,j}$, we calculate the following points:

$$(13) \quad t_{i,j} = (g_{i,j}, q_{i,j}) / (q_{i,j}, Aq_{i,j}) \quad \text{or} \quad t_{i,j} = (g_{i,j}, Kg_{i,j}) / (q_{i,j}, Aq_{i,j}),$$

$$(14) \quad p_{i,j+1} = p_{i,j} + t_{i,j}q_{i,j},$$

$$(15) \quad r_{i,j+1} = r_{i,j} - t_{i,j} N q_{i,j},$$

$$(16) \quad g_{i,j+1} = N^* H r_{i,j+1},$$

$$(17) \quad s_{i,j} = -(A q_{i,j}, K g_{i,j+1}) / (q_{i,j}, A q_{i,j}) \quad \text{or} \quad s_{i,j} = (g_{i,j+1}, K g_{i,j+1}) / (g_{i,j}, K g_{i,j}),$$

$$(18) \quad q_{i,j+1} = K g_{i,j+1} + s_{i,j} q_{i,j},$$

$$(19) \quad g_{i,j+1} = g_{i,j} - t_{i,j} A q_{i,j}.$$

The above algorithm is in fact the conjugate gradient method applied to the linear system for the unknowns p_i with respect to given x_i :

$$(20) \quad N p_i = M^* x_i - \mu(x_i) N x_i.$$

The algorithm (10) to (19) follows the Hestenes' order. After [1], there exists a positive integer $m_i \leq n$ such that

$$(21) \quad 0 = g_{i,m_i} = A(h_i - p_{i,m_i}), \quad h_i = N^{-1}(M^* x_i - \mu(x_i) N x_i).$$

Now we put

$$(22) \quad p_i = p_{i,m_i}.$$

Then the iteration goes in the following order:

$$(23) \quad x_{i+1} = x_i + a p_i, \quad (a \text{ being a suitable fixed constant})$$

$$(24) \quad \lambda_{i+1} = \mu(x_{i+1}).$$

$$(25) \quad \begin{array}{ccccccc} x_0 & \xrightarrow{T_0} & p_0 & \longrightarrow & x_1 & \xrightarrow{T_1} & \cdots \longrightarrow x_i & \xrightarrow{T_i} & p_i & \longrightarrow & x_{i+1} & \xrightarrow{T_{i+1}} & p_{i+1} & \longrightarrow & \cdots \longrightarrow \cdots \\ \mu \downarrow & & & & \mu \downarrow & & & & \mu \downarrow & & \mu \downarrow & & & & \\ \lambda_0 & \longrightarrow & \lambda_1 & \longrightarrow & \cdots & \longrightarrow & \lambda_i & \longrightarrow & \lambda_{i+1} & \longrightarrow & \cdots & \longrightarrow & \cdots \end{array}$$

where $T_i = N^{-1}(M^* - \mu(x_i)N)$ which depends on x_i .

$$(26) \quad \begin{array}{ccccccc} y_0 = (x_0, \lambda_0) & \longrightarrow & y_1 = (x_1, \lambda_1) & \longrightarrow & \cdots & \longrightarrow & \cdots \\ & & \longrightarrow & y_i = (x_i, \lambda_i) & \longrightarrow & y_{i+1} = (x_{i+1}, \lambda_{i+1}) & \longrightarrow \cdots \longrightarrow \cdots \end{array}$$

We have

LEMMA 1. *If the matrix M is Hermitian, then the following relations (27)–(31) hold.*

$$(27) \quad (N p_i, x_i) = 0 \quad \text{for all } x_i \text{ and } p_i,$$

i. e. x_i and p_i are N -orthogonal, so the point x_{i+1} lies in the N -orthogonal direction of the vector x_i in the space V^n .

$$(28) \quad (p_i, M x_i) = (p_i, N p_i) \quad \text{for all } x_i \text{ and } p_i,$$

i. e. $(p_i, M x_i)$ is a real number and is equal to the square of N -norm of p_i .

$$(29) \quad (Nx_{i+1}, x_i) = (Nx_i, x_i),$$

$$(30) \quad (Np_i, x_{i+k}) = a \sum_{j=0}^{k-1} (Np_i, p_{i+j}), \quad (k \geq 1),$$

$$(31) \quad (Nx_j, x_j) = (Nx_i, x_i) + a^2 \sum_{l=i}^{j-1} (Np_l, p_l), \quad (j > i).$$

PROOF. From (20) and $M = M^*$, we get

$$\begin{aligned} (Np_i, x_i) &= (Mx_i - \mu(x_i)Nx_i, x_i) \\ &= (Mx_i, x_i) - \mu(x_i)(Nx_i, x_i) = 0 \quad \text{for all } x_i \text{ and } p_i. \\ (p_i, Mx_i) &= (p_i, Np_i) + \mu(x_i)(p_i, Nx_i) = (p_i, Np_i) \quad (\text{by (27)}). \end{aligned}$$

Using the result of (27),

$$(Nx_{i+1}, x_i) = (Nx_i, x_i) + a(Np_i, x_i) = (Nx_i, x_i).$$

When $k=1$, (30) holds. In fact we have

$$(Np_i, x_{i+1}) = (Np_i, x_i) + a(Np_i, p_i) = a(Np_i, p_i) \quad \text{by (27)}.$$

Assume the relation (30) for $k=l$. Then for $k=l+1$, we get

$$\begin{aligned} (Np_i, x_{i+l+1}) &= (Np_i, x_{i+l}) + a(Np_i, p_{i+l}) \\ &= a \sum_{j=0}^{l-1} (Np_i, p_{i+j}) + a(Np_i, p_{i+l}) \\ &= a \sum_{j=0}^l (Np_i, p_{i+j}). \end{aligned}$$

In the same way (31) may be proved by induction.

THEOREM 1. *If M is an Hermitian matrix and a is a fixed number (positive or negative) such that*

$$(32) \quad |a| < D,$$

where $D = 1/(\hat{\lambda}_{\max} - \hat{\lambda}_{\min})$, $\hat{\lambda}_{\max}$ and $\hat{\lambda}_{\min}$ being, respectively, the maximum and the minimum eigenvalue of (1), then the algorithm (10)–(24) gives the numerical solution for the eigenvalues $\hat{\lambda}_1, \hat{\lambda}_2, \dots, \hat{\lambda}_n$ of (1).

REMARK. The condition for M is satisfied, for example, either when B and H are both identity matrix or when B is real symmetric and $H = B^{-1}$.

PROOF. From the definition of $\mu(x)$ and the condition for M , we get the formula:

$$\begin{aligned} \mu(x_{i+1}) &= (M(x_i + ap_i), x_i + ap_i) / (x_{i+1}, Nx_{i+1}) \\ &= \{(Mx_i, x_i) + a(Mp_i, x_i) + a(Mx_i, p_i) + a^2(Mp_i, p_i)\} / (x_{i+1}, Nx_{i+1}) \end{aligned}$$

$$\begin{aligned}
&= \{(Mx_i, x_i) + 2a(p_i, Np_i) + a^2(Mp_i, p_i)\} / (x_{i+1}, Nx_{i+1}) \\
&= \{(Mx_i, x_i) + 2a(p_i, Np_i) + a^2\mu(p_i)(p_i, Np_i)\} / (x_{i+1}, Nx_{i+1}) . \\
(33) \quad \mu(x_{i+1}) &= \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} \left\{ \frac{(Mx_i, x_i)}{a(p_i, Np_i)} + 2 + a\mu(p_i) \right\} .
\end{aligned}$$

And now

$$\mu(x_i) = \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} \frac{(x_{i+1}, Nx_{i+1})}{(x_i, Nx_i)} \frac{(Mx_i, x_i)}{a(p_i, Np_i)}$$

and

$$\begin{aligned}
\frac{(x_{i+1}, Nx_{i+1})}{(x_i, Nx_i)} &= \frac{1}{(x_i, Nx_i)} \{(x_i, Nx_i) + a(p_i, Nx_i) + a(x_i, Np_i) + a^2(p_i, Np_i)\} \\
(34) \quad &= 1 + \frac{a^2(p_i, Np_i)}{(x_i, Nx_i)} .
\end{aligned}$$

Hence

$$(35) \quad \mu(x_i) = \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} \left\{ \frac{(Mx_i, x_i)}{a(p_i, Np_i)} + a\mu(x_i) \right\} .$$

From (33) and (35) follows

$$(36) \quad \mu(x_{i+1}) - \mu(x_i) = \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} [a\{\mu(p_i) - \mu(x_i)\} + 2] .$$

Hence

$$(37) \quad \lambda_{i+1} - \lambda_i = \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} [2 + a(\mu(p_i) - \lambda_i)] .$$

By this formula the convergence of the sequence $\{\lambda_i\}$ may be proved under the assumption for a . In fact any $x \in V^n$ being represented by the eigenvectors $\hat{x}_1, \hat{x}_2, \dots, \hat{x}_n$, where $\hat{x}_j$ is the normalized eigenvector corresponding to the eigenvalue $\hat{\lambda}_j$, i. e.,

$$(38) \quad x = \sum_{k=1}^n c_k \hat{x}_k, \quad c_k = (x, \hat{x}_k),$$

we have

$$(39) \quad \hat{\lambda}_{\min} \leq \mu(x) = \frac{\sum_{i,j=1}^n c_i c_j (M\hat{x}_i, \hat{x}_j)}{\sum_{i,j=1}^n c_i c_j (\hat{x}_i, N\hat{x}_j)} \leq \hat{\lambda}_{\max} .$$

Hence

$$(40) \quad |a(\mu(p_i) - \lambda_i)| < D(\hat{\lambda}_{\max} - \hat{\lambda}_{\min}) = 1$$

and

$$(41) \quad 2 + a(\mu(p_i) - \lambda_i) > 0 \quad \text{for all } p_i \text{ and } \lambda_i.$$

If a is positive in the range (32) the sequence $\{\lambda_i\}$ is monotone increasing, and if a is negative it is monotone decreasing.

As the sequence $\{\lambda_i\}$ is bounded and monotone, it converges to some value between $\hat{\lambda}_{\min}$ and $\hat{\lambda}_{\max}$. The convergence is, in fact, guaranteed even under the weaker condition

$$(42) \quad |a| < 2D.$$

For we have then

$$(43) \quad |a(\mu(p_i) - \lambda_i)| < 2D(\hat{\lambda}_{\max} - \hat{\lambda}_{\min}) = 2,$$

hence (41) holds.

To complete the proof of the theorem, we need the following

LEMMA 2. *The above mentioned sequence $\{x_i\}$ has a non-zero accumulation point and it is unique.*

PROOF. It is sufficient to prove that

$$(44) \quad x_{i+1} \neq 0 \quad \text{for all } i,$$

when $\|x_i\| = 1$. In fact, if this is true, the sequence $\{\tilde{x}_i\}$, $\tilde{x}_i$ being the normalized vector corresponding to the vector x_i , has an accumulation point on the unit sphere $\|x\| = 1$. And since (20) and (23) are homogeneous with respect to x_i and p_i , we can drop the condition $\|x\| = 1$. To prove (44), we must calculate Bp_i . From (20) and the condition of the theorem, we get

$$(45) \quad Bp_i = (A - \mu(x_i)B)x_i,$$

and

$$(46) \quad p_i = B^{-1}(A - \mu(x_i)B)x_i,$$

so that (44) reduces to

$$(47) \quad x_i + aB^{-1}(A - \mu(x_i)B)x_i \neq 0,$$

i. e.

$$(48) \quad aB^{-1}(A+(1/a-\mu(x_i))B)x_i \neq 0 \quad \text{for all } x_i.$$

Hence it is necessary and sufficient that the matrix $A+(1/a-\mu(x_i))B$ is non-singular. If a is so taken as to satisfy the inequality

$$(49) \quad \hat{\lambda}_{\min}-1/a > \hat{\lambda}_{\max} \quad \text{or}$$

$$(50) \quad \hat{\lambda}_{\max}-1/a < \hat{\lambda}_{\min},$$

then from the relation

$$(51) \quad \hat{\lambda}_{\min}-1/a \leq \mu(x_i)-1/a \leq \hat{\lambda}_{\max}-1/a$$

follows that the matrix $A+(1/a-\mu(x_i))B$ is non-singular.

The condition (49) or (50) determines the range for a :

$$(52) \quad 0 < |a| < 1/(\hat{\lambda}_{\max}-\hat{\lambda}_{\min}) = D.$$

Now the number a in the theorem being determined so as to satisfy (52), we have thus proved (44). The uniqueness is proved easily. Accordingly we obtain the lemma.

Thus the iterative sequence $\{x_i\}$ has a non zero accumulation point, so that for a suitable subsequence it holds $\lim_{i \rightarrow \infty} x_{i_\nu} = x_\infty (\neq 0)$.

We shall next show, by means of the foregoing lemma, that the point $y = (x_\infty, \lim_{i \rightarrow \infty} \mu(x_{i_\nu}))$ is one of the eigenpoints for (1). The convergence of $\{\lambda_i\}$ implies that to any positive quantity ε the inequality

$$(53) \quad |\lambda_{i+1} - \lambda_i| < \varepsilon, \quad i > R(\varepsilon)$$

holds, if a positive integer $R(\varepsilon)$ is chosen sufficiently large. Thus, by (37), to an arbitrary $\varepsilon_1 > 0$, it holds

$$(54) \quad (p_{i_\nu}, Np_{i_\nu})/(x_{i_\nu+1}, Nx_{i_\nu+1}) < \varepsilon_1, \quad i_\nu > R_1(\varepsilon_1).$$

As (x_∞, Nx_∞) is neither zero nor infinity by the lemma 2, to any positive ε_2 we have

$$(55) \quad (p_{i_\nu}, Np_{i_\nu}) < \varepsilon_2, \quad i_\nu > R_2(\varepsilon_2).$$

Combined with the property of N , to any positive ε_3 , it holds

$$(56) \quad (p_{i_\nu}, p_{i_\nu}) < \varepsilon_3, \quad i_\nu > R_3(\varepsilon_3).$$

The relation (56) implies that

$$(57) \quad p_{i_\nu} \rightarrow 0 \quad \text{as } \nu \rightarrow \infty.$$

Hence we have

$$(58) \quad Np_{i_\nu} \rightarrow 0 \quad \text{as } \nu \rightarrow \infty ,$$

and

$$(59) \quad Np_{i_\nu} = Mx_{i_\nu} - \mu(x_{i_\nu})Nx_{i_\nu} \rightarrow Mx_\infty - \{\lim_{\nu \rightarrow \infty} \mu(x_{i_\nu})\}Nx_\infty \quad \text{as } \nu \rightarrow \infty .$$

From the relations (58) and (59) we get

$$(60) \quad Mx_\infty - \{\lim_{\nu \rightarrow \infty} \mu(x_{i_\nu})\}Nx_\infty = 0 ,$$

i. e.

$$(61) \quad B^*H(Ax_\infty - \{\lim_{\nu \rightarrow \infty} \mu(x_{i_\nu})\}Bx_\infty) = 0 .$$

As B^* is non-singular and H is positive Hermitian,

$$(62) \quad Ax_\infty = \{\lim_{\nu \rightarrow \infty} \lambda_{i_\nu}\}Bx_\infty .$$

This shows that $y = (x_\infty, \lim_{\nu \rightarrow \infty} \lambda_{i_\nu})$ is some eigenpoint for (1) in the space $V^n \times C$. Now by selecting other suitable points x as starting points and proceeding in the same way as above, we may get the other eigenpoints.

REMARK 1. The eigenvector can be calculated by other methods if the eigenvalue is found. In using this algorithm, the freedom of the selection of the quantity a will be greater the smaller the distance between $\hat{\lambda}_{\min}$ and $\hat{\lambda}_{\max}$ is.

REMARK 2. From the hypothesis in theorem 1 the formula (20) becomes

$$(20)' \quad Bp_i = Ax_i - \mu(x_i)Bx_i$$

and thus the algorithm for computing p_i is simplified as follows. In this case,

$$A \equiv N = B^*HB ,$$

$$(10)' \quad r_{i,0} = Ax_i - \mu(x_i)Bx_i - Bp_{i,0} ,$$

$$(11)' \quad g_{i,0} = B^*Hr_{i,0} \quad (= Mx_i - \mu(x_i)Nx_i - Np_{i,0}) ,$$

$$(12)' \quad q_{i,0} = Kg_{i,0} ,$$

$$(13)' \quad t_{i,j} = (g_{i,j}, q_{i,j}) / (q_{i,j}, Nq_{i,j}) \quad \text{or}$$

$$t_{i,j} = (g_{i,j}, Kg_{i,j}) / (q_{i,j}, Nq_{i,j}) ,$$

$$(14)' \quad p_{i,j+1} = p_{i,j} + t_{i,j}q_{i,j} ,$$

$$\begin{aligned}
(15)' \quad & r_{i,j+1} = r_{i,j} - t_{i,j} B q_{i,j}, \\
(16)' \quad & g_{i,j+1} = B^* H r_{i,j+1}, \\
(17)' \quad & s_{i,j} = -(B q_{i,j}, K g_{i,j+1}) / (q_{i,j}, N q_{i,j}) \quad \text{or} \\
& s_{i,j} = (g_{i,i+1}, K g_{i,j+1}) / (g_{i,j}, K g_{i,j}), \\
(18)' \quad & q_{i,j+1} = K g_{i,j+1} + s_{i,j} q_{i,j}, \\
(19)' \quad & g_{i,j+1} = g_{i,j} - t_{i,j} N q_{i,j}.
\end{aligned}$$

We notice that in this case we shall reach a similar conclusion when we use as the direction vector;

$$(63) \quad p_i = T(Ax_i - \mu(x_i)Bx_i),$$

where T is a given matrix. (When $T=B^{-1}$, the algorithm is just the one in the theorem 1.)

Corresponding to (63) we may take the following p_i ;

$$(64) \quad T p_i = M^* x_i - \mu(x_i) N x_i,$$

T being a positive definite Hermitian matrix and satisfying the inequality

$$(65) \quad 0 < T < N$$

in the sense of a linear operator in the space V^n , i. e.:

$$(66) \quad 0 < (p, T p) < (p, N p) \quad \text{for all } p \in V^n.$$

In this case, a similar theorem is obtained as a corollary of the theorem 1.

THEOREM 2. *Let the eigenvalues for (1) be all real and distinct, and M be Hermitian. Then the iteration*

$$(67) \quad \begin{cases} T p_i = M^* x_i - \mu(x_i) N x_i, & (i=0, 1, 2, \dots), \\ x_{i+1} = x_i + a p_i, \\ \lambda_{i+1} = \mu(x_{i+1}) \end{cases}$$

gives an eigenvalue for (1) as $\lim_{i \rightarrow \infty} \lambda_i$, when T is a positive definite Hermitian matrix having the property (65) and a is a negative quantity satisfying the condition

$$(68) \quad -1/(\hat{\lambda}_{\max} - \hat{\lambda}_{\min}) < a < 0.$$

PROOF. By simple calculation we get

$$\begin{aligned}
(69) \quad \mu(x_{i+1}) - \mu(x_i) = & \frac{a(p_i, N p_i)}{(x_{i+1}, N x_{i+1})} [a\{\mu(p_i) - \mu(x_i)\} \\
& + 1/(p_i, N p_i)\{(p_i, M x_i - \mu(x_i) N x_i) + (x_i, M p_i - \mu(x_i) N p_i)\}].
\end{aligned}$$

p_i being the solution of the first equation of (67) and $M^*=M$, we get

$$(70) \quad \mu(x_{i+1}) - \mu(x_i) = \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} \left[a\{\mu(p_i) - \mu(x_i)\} + \frac{1}{(p_i, Np_i)} \{(p_i, Tp_i) + (Tp_i, p_i)\} \right].$$

By the condition (65) we have

$$(71) \quad \mu(x_{i+1}) - \mu(x_i) \leq \frac{a(p_i, Np_i)}{(x_{i+1}, Nx_{i+1})} [a\{\mu(p_i) - \mu(x_i)\} + 2] \leq 0.$$

The sequence $\{\lambda_i\}$ is monotone decreasing. The remaining part of the proof is similar to the theorem 1.

References

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