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THE EIGENVALUES OF A FULL SYMMETRIC MATRIX -
AN ALTERNATIVE TO JACOBI'S METHOD

T. Nanda

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THE EIGENVALUES OF A FULL SYMMETRIC MATRIX - AN ALTERNATIVE TO JACOBI'S METHOD[1]

T. Nanda

Department of Mathematics
and
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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Abstract: The algorithm described in this article uses Householder reflections to obtain the largest eigenvalue of a full positive definite matrix. The method is a special case of the power method but has several interesting features. The algorithm can be used to obtain all the eigenvalues of a symmetric matrix and is eminently suitable for a parallel processing machine. For such machines this method should be much better as compared to the Jacobi's method. The algorithm has a built in deflation and has a reliable stopping criterion. We also consider the differential equations analogue of this method and prove the convergence of that method together with the convergence rates. Finally some numerical examples are given.

1. Introduction

Let A be an $n \times n$ positive definite matrix with eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \ldots < \lambda_n$. In this paper we describe a method to obtain the eigenvalues of A and in particular the largest eigenvalue of A, or the first few largest ones. The basic idea is to apply a sequence of reflections so that in the limit the first column of the matrix A converges to a multiple of $e_1 = (1,0,0, \ldots, 0)^T$. A similar idea has been considered by LaBudde in [1] where the author uses both Householder reflections and Jacobi rotations in succession to achieve the same effect on the matrix A. Our method is a special case of the power method where the starting vector is e_1. As a consequence the method converges linearly with convergence ratio $\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^2$ In contrast to the power method itself, this method transforms the matrix A at each step, as a result the convergence can be accelerated by means of shifts, or by Aitken's procedure or both. As is well known, to implement shifts in the power method is not well suited for automatic computation. Moreover this algorithm has a reliable and economical stopping criterion. From this point of view this method is suggested as a rival to the Lanczos algorithm considered by the authors in [7].

The Jacobi method [4] for finding the eigenvalues of a full symmetric matrix is well suited for sequential machines. The algorithm presented in this paper should perform equally well. However the present algorithm is eminently suitable for a parallel processing machine and should be superior to Jacobi's method on such machines.

We also consider the differential equations analogue (see [6]) of this method. Here the general idea is to write down a system of equations:

$$\frac{dL}{dt} = B(t)L(t) - L(t)B(t)$$

(1)

$$L(0) = A$$

where $B(t)$ is a skew symmetric matrix of order n. This system, for suitable choices of B, converges as $t \to +\infty$ to a limit matrix A_∞ which has the same set of eigenvalues as A. If B is taken to be the matrix

$$B = \begin{pmatrix} 0 & b^T \\ b & 0 \end{pmatrix}$$

where (a_1, b^T) is the first row of $L(t)$, then as $t \to \infty$ the matrix $L(t)$ converges to a matrix of the form A_∞ where

$$A_\infty = \begin{pmatrix} \lambda & 0 \\ 0 & M_\infty \end{pmatrix}$$

and λ is an eigenvalue of A. Generically λ is equal to the largest eigenvalue λ_n of A. The system (1) is also suitable for parallel processors and could be used to solve the eigenvalue problem.

The study of the system (1) has been done in [2], [3], [6] and the connection of (1) with the QR algorithm fully investigated in [5], [6]. This system has also been used for numerical computations of eigenvalues in [8], [9].

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2. Description of the algorithm; Definition and notations

Let $A \equiv (a_{jk})$ be a positive definite matrix of order n. We shall write

$$A = \begin{pmatrix} a_1 & b^T \\ b & M \end{pmatrix}$$

where $a_1 = a_{11}$, b is a n-1 vector and M is a positive definite matrix of order n-1. We denote by U_0 an orthonormal matrix consisting of the eigenvectors of A and by $\Lambda \equiv \mathrm{diag}[\lambda_1, \ldots, \lambda_n]$ the matrix of the eigenvalues arranged so that $0 < \lambda_1 \leq \lambda_2 \leq \ldots\ldots < \lambda_n$. We can therefore write

$$A = U_0 \Lambda U_0^T .$$

The vector $U_0{}^T e_1$ will be denoted by f_0. In section 6 we shall denote by $f(t)$ the vector $U^T(t)e_1$ where $U(t)$ is the matrix of eigenvectors for the matrix $L(t)$ which satisfies (1).

The algorithm is defined as follows: starting with A we apply an orthogonal transformation $H_0(u\ )$ and define A_1 by

$$A_1 = H_0(u)AH_0(u)$$

where

$$H_0(u) = I - \frac{2u\ u^T}{\|u\|^2}$$

and the vector u is chosen so that $H_0(u)$ transforms the vector $(a_1, b^T)^T$ into $-\sqrt{a_1^2 + \|b\|^2}\ e_1$. As is well known (see e.g. [4]) we can write

$$u = \left(a_1 + \sqrt{a_1^2 + \|b\|^2}\ ,\ b^T\right)^T.$$

The process is repeated indefinitely and we will show that in the limit we obtain a matrix of the form

$$\begin{pmatrix} \lambda & 0 \\ 0 & M_\infty \end{pmatrix}$$

At a typical stage we have

$$A_{m+1} = \begin{pmatrix} a_1(m+1) & b^T(m+1) \\ b(m+1) & M(m+1) \end{pmatrix} = H_m A_m H_m$$

where

$$H_m = I - \gamma_m\ u(m)u^T(m) \quad ,$$

$$\gamma_m = \frac{2}{\|u(m)\|^2} \ ,$$

$$u^T(m) = \left(a_1(m) + \sqrt{a_1^2(m) + \|b(m)\|^2}\ ,\ b^T(m)\right) .$$

We will show that $\|b(m)\|^2 \to 0$ as $m \to \infty$ so this method provides a very reliable and economical criterion to deflate the matrix.

3. Proof of the convergence of the algorithm

The following facts are easily verified:

(i) $$\gamma_m^{-1} = \sqrt{a_1^2(m) + \|b(m)\|^2}\left(a_1(m) + \sqrt{a_1^2(m) + \|b(m)\|^2}\right)$$

(ii) $$H_m = \begin{pmatrix} \dfrac{-a_1(m)}{\sqrt{a_1^2(m) + \|b(m)\|^2}} & \dfrac{-b^T(m)}{\sqrt{a_1^2(m) + \|b(m)\|^2}} \\ \dfrac{-b\ (m)}{\sqrt{a_1^2(m) + \|b(m)\|^2}} & I - \gamma_m b(m) b^T(m) \end{pmatrix}$$

(iii) $$a_1(m+1) = a_1(m) + \frac{a_1(m)\|b(m)\|^2 + b^T(m)M(m)b(m)}{a_1^2(m) + \|b(m)\|^2}$$

<u>Theorem 1</u>. $\lim_{m\to\infty} a_1(m) = \lambda$ exists and is an eigenvalue of A. Moreover if $e_n^T f_0 \neq 0$ then $\lambda = \lambda_n$; if in addition $e_{n-1}^T f_0 \neq 0$ then

$$\lim_{m\to\infty}\left|\frac{a_1(m+1) - \lambda}{a_1(m) - \lambda}\right| = \left(\frac{\lambda_{n-1}}{\lambda_n}\right)^2 .$$

<u>Proof</u>. From (iii) above $a_1(m+1) \geq a_1(m)$ because A_m is positive definite. Thus the sequence $\{a_1(m)\}$ is a monotonically increasing sequence bounded from above by $\|A\|$. It follows that $\lim_{m\to\infty} a_1(m) = \lambda$ exists and from (iii) it follows that $\lim_{m\to\infty} \|b(m)\|^2 = 0$. Let $U_m = H_{m-1}U_{m-1}$ denote the matrix of the eigenvectors of A_m, and let $f_m = U_m^T e_1$.

Then $f_1 = U_1^T e_1 = (H_0 U_0)^T e_1 = U_0^T H_0 e_1$. From (ii)

$$H_0 e_1 = -\frac{Ae_1}{\|Ae_1\|}$$

so that

$$f_1 = -\frac{U_0^T A e_1}{\|Ae_1\|} = -\frac{\Lambda U_0^T e_1}{\|U_0 \Lambda U_0^T e_1\|} = -\frac{\Lambda f_0}{\|\Lambda f_0\|}$$

By induction it follows that

$$f_m = (-1)^m \frac{\Lambda^m f_0}{\|\Lambda^m f_0\|}$$

By hypotheses $e_n^T f_0 \neq 0$ so

$$(-1)^m f_m \to (0, 0, \ldots 1)^T.$$

Since $\|f_m\| = 1$ and $a_1(m) = f_m^T \Lambda f_m$ it follows that

$$\lim_{m\to\infty} a_1(m) = \lambda_n$$

and if $e_{n-1}^T f_0 \neq 0$ then

$$\lim_{m\to\infty} \left| \frac{a_1(m) - \lambda_n}{a_1(m-1) - \lambda_n} \right| = \left(\frac{\lambda_{n-1}}{\lambda_n} \right)^2 .$$

Remark. In [1] the author does not have an exact theoretical rate of convergence.

4. Connection with the Power method

Consider the power method defined below:

$$x_0 = e_1 \quad \text{and for} \quad m \geq 1$$

$$x_m = \frac{Ax_{m-1}}{\|Ax_{m-1}\|} \quad , \quad \rho_m = x_m^T A x_m \ .$$

The next lemma shows that the Rayleigh quotient ρ_m is equal to $a_1(m)$.

Lemma. (i) $x_m = (-1)^m H_0 H_1 \ldots H_{m-1} e_1$

(ii) $a_1(m) = \rho(m)$

for every $m \geq 1$.

Proof:

$$x_1 = \frac{Ae_1}{\|Ae_1\|} = -H_0 e_1$$

$$\rho_1 = x_1^T A x_1$$

$$= e_1^T H_0 A H_0 e_1$$

$$= e_1^T A_1 e_1$$

$$= a_1(1)$$

so the lemma is true for $m = 1$.

Assume the result is true for m. We will prove it for $m + 1$. By induction hypothesis

$$x_m = (-1)^m H_0 H_1 \ldots H_{m-1} e_1$$

so

$$\begin{aligned} Ax_m &= (-1)^m A H_0 H_1 \ldots H_{m-1} e_1 \\ &= (-1)^m H_0 A_1 H_1 \ldots H_{m-1} e_1 \\ &= \ldots\ldots \\ &= (-1)^m H_0 H_1 \ldots H_{m-1} A_m e_1 \\ &= (-1)^m H_0 H_1 \ldots H_{m-1} (-\|A_m e_1\| H_m e_1) \\ &= (-1)^{m+1} \|A_m e_1\| \, H_0 H_1 \ldots H_m e_1 \end{aligned}$$

and $\|Ax_m\| = \|A_m e_1\|$. Hence

$$x_{m+1} = \frac{Ax_m}{\|Ax_m\|} = (-1)^{m+1} H_0 H_1 \ldots H_m e_1$$

Finally

$$\begin{aligned} \rho_{m+1} &= x_{m+1}^T A x_{m+1} \\ &= e_1^T H_m H_{m-1} \ldots H_0 A H_0 H_1 \ldots H_m e_1 \end{aligned}$$

$$= e_1^T A_{m+1} e_1$$

$$= a_1(m+1)$$

and the proof is complete.

Remark. In view of the above Lemma it is not surprising that the method described in section 2 converges linearly with convergence ratio $\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^2$.

5. Numerical results

We give here the numerical results for matrices of order 6×6. All computations were done in single precision on the Vax at the University of California, Berkeley.

Example 1. Here we consider a 6×6 Hilbert matrix $A \equiv (a_{ij})$ defined by $a_{ij} = \frac{1}{i+j-1}$.

In Table1we present a snapshot of the matrices $A_1, A_2, A_3, A_4, \ldots$ The convergence to the largest eigenvalue is quite fast as can be seen from the fact that $\|b\|^2$ decreases to zero rapidly.

Example 2. This example was designed to show the effect of the shifts. A reasonable choice of the shift is $\sigma = \frac{\lambda_1 + \lambda_{n-1}}{2}$. In the present example the eigenvalues are close to successive integers with $\lambda_n \approx 10$ and $\lambda_{n-1} \approx 9$. We arrange the matrix A so that $a_{11} \geq a_{22} \geq \cdots \geq a_{66}$ and after k-th iteration use the shift

$$\sigma_k = \frac{a_{22}(k) + a_{66}(k)}{2}$$

$$A = \begin{pmatrix} 10 & 1 & .5 & .25 & .125 & .1 \\ 1 & 9 & .4 & .2 & .1 & .05 \\ .5 & .4 & 8 & .3 & .15 & .1 \\ .25 & .2 & .3 & 7 & .5 & .4 \\ .125 & .1 & .15 & .5 & 6 & 1 \\ .1 & .05 & .1 & .4 & 1 & 5 \end{pmatrix}$$

Without shifts at the end of 20 iterations we have

$$A_{20} = \begin{pmatrix} 10.822784 & +0.009937 & 0.003310 & 0.001418 & 0.000771 & 0.000467 \\ 0.009937 & 8.365804 & 0.100468 & 0.055740 & 0.024034 & -0.003446 \\ 0.003310 & 0.100468 & 7.858157 & 0.231583 & 0.114022 & 0.074598 \\ 0.001418 & 0.055740 & 0.231583 & 6.966969 & 0.482646 & 0.387721 \\ 0.000771 & 0.024034 & 0.114022 & 0.482646 & 5.990870 & 0.993558 \\ 0.000467 & -0.003446 & 0.74598 & 0.387721 & 0.993558 & 4.995424 \end{pmatrix}$$

If we use shifts then at the end of 7 iterations one gets

$$A_7 = \begin{pmatrix} 10.822808 & -0.005729 & -0.001641 & -0.000691 & -0.000199 & -0.000517 \\ -0.005729 & 8.365579 & 0.100637 & 0.056086 & 0.023938 & -0.003039 \\ -0.001641 & 0.100637 & 7.858235 & 0.231712 & 0.113968 & 0.074769 \\ -0.000691 & 0.056086 & 0.231712 & 6.967099 & 0.482642 & 0.387812 \\ -0.000199 & 0.023938 & 0.113968 & 0.482642 & 5.990872 & 0.993588 \\ -0.000517 & -0.003039 & 0.074769 & 0.387812 & 0.993588 & 4.995508 \end{pmatrix}$$

TABLE 1

$$A_1 = \begin{pmatrix} 1.598409 & -0.067169 & -0.081336 & -0.079618 & -0.074553 & -0.069045 \\ -0.067169 & 0.047670 & 0.051330 & 0.046807 & 0.041668 & 0.037134 \\ -0.081336 & 0.051330 & 0.062067 & 0.060424 & 0.056233 & 0.051775 \\ -0.079618 & 0.046807 & 0.060424 & 0.061079 & 0.058356 & 0.054795 \\ -0.074553 & 0.041668 & 0.056233 & 0.058356 & 0.056818 & 0.054133 \\ -0.069045 & 0.037134 & 0.051775 & 0.054795 & 0.054133 & 0.052167 \end{pmatrix}$$

$$A_2 = \begin{pmatrix} 1.618435 & 0.009656 & 0.012166 & 0.012175 & 0.011572 & 0.010836 \\ 0.009656 & 0.044442 & 0.047410 & 0.042965 & 0.038067 & 0.033796 \\ 0.012166 & 0.047410 & 0.057310 & 0.055760 & 0.051861 & 0.047723 \\ 0.012175 & 0.042965 & 0.055760 & 0.056507 & 0.054070 & 0.050823 \\ 0.011572 & 0.038067 & 0.051861 & 0.054070 & 0.052801 & 0.050410 \\ 0.010836 & 0.033796 & 0.047723 & 0.050823 & 0.050410 & 0.048717 \end{pmatrix}$$

$$A_3 = \begin{pmatrix} 1.618890 & -0.001440 & -0.001820 & -0.001824 & -0.001736 & -0.001626 \\ -0.001440 & 0.044376 & 0.047327 & 0.042881 & 0.037987 & 0.033722 \\ -0.001820 & 0.047327 & 0.057204 & 0.055654 & 0.051761 & 0.047630 \\ -0.001824 & 0.042881 & 0.055654 & 0.056402 & 0.053970 & 0.050730 \\ -0.001736 & 0.037987 & 0.051761 & 0.053970 & 0.052706 & 0.050321 \\ -0.001626 & 0.033722 & 0.047630 & 0.050730 & 0.050321 & 0.048633 \end{pmatrix}$$

$$A_4 = \begin{pmatrix} 1.61890 & 0.000216 & 0.000272 & 0.000273 & 0.000260 & 0.000244 \\ 0.000216 & 0.044374 & 0.047325 & 0.042879 & 0.037986 & 0.033720 \\ 0.000272 & 0.047325 & 0.057202 & 0.055652 & 0.051759 & 0.047627 \\ 0.000273 & 0.042879 & 0.055652 & 0.056400 & 0.053968 & 0.050728 \\ 0.000260 & 0.037986 & 0.051759 & 0.053968 & 0.052704 & 0.050319 \\ 0.000244 & 0.033720 & 0.047627 & 0.050728 & 0.050319 & 0.048631 \end{pmatrix}$$

5. The point of view of differential equations

In this section we consider the system of differential equations

$$(*) \qquad \begin{cases} \dfrac{dL}{dt} = B(t)L(t) - L(t)B(t) \\ L(0) = A \end{cases}$$

where we write

$$L(t) = \begin{pmatrix} a_1(t) & b^t(t) \\ b(t) & M(t) \end{pmatrix}$$

and

$$B(t) = \begin{pmatrix} 0 & b^T(t) \\ -b(t) & 0 \end{pmatrix}$$

is a $n \times n$ skew symmetric matrix.

Theorem 2. Let $L(t)$ be the solution of the system (*). Then

(i) $L(t)$ has the same eigenvalues as A for all times

(ii) $L(t)$ converges to $\begin{pmatrix} \lambda & 0 \\ 0 & M_\infty \end{pmatrix}$ as $t \to \infty$

(iii) If $e_n^T f_0 \neq 0$ then λ is the largest eigenvalue λ_n of A.

Remarks 1. The algoirthm described in section (2) is a discrete analogue of the system (*).

2. We shall call the flow defined by (*) as a "deflator" since it deflates the matrix.

Proof of Theorem 2. From the theory of ordinary differential equations the system (*) has a solution which exists for some time interval $(-\varepsilon, \varepsilon)$. Let $U(t)$ be defined by

$$(**) \qquad \begin{cases} \frac{d}{dt} U(t) = B(t)U(t) \\ U(0) = I \end{cases} \qquad t \in (-\varepsilon, \varepsilon)$$

we have

$$\frac{d}{dt}(U^T U) = -U^T BU + U^T BU = 0$$

so $U(t)$ is unitary for $t \in (-\varepsilon,\varepsilon)$. Next $\frac{d}{dt}(U^t(t)L(t)U(t)) = 0$ so that

$$L(t) = U(t)L(0)U^T(t) = U(t)AU^T(t).$$

Thus $L(t)$ has the same eigenvalues as A and $\|L(t)\| = \|A\|$. This implies that the system (*) has a solution existing for all times. From (*) we get

(1) $\frac{da_1}{dt} = 2\|b(t)\|^2$

(2) $\frac{db}{dt} = M(t)b(t) - a_1(t)b(t)$

(3) $\frac{dM}{dt} = -2b(t)b^T(t).$

Equation (1) together with the fact that $\|L(t)\| = \|A\|$ implies that

(4) $$\int_{-\infty}^{\infty} \|b(s)\|^2 \, ds < \infty.$$

Equation (2) implies that $\left|\frac{d}{dt} b_j(t)\right|$ is bounded for all times so that

(5) $\quad |\|b(t_1)\| - \|b(t_2)\|| \leq K|t_1-t_2|$

for some constant K independent of t_1 and t_2. We now assert that $\|b(s)\|$ converges to 0 as $s \to \infty$. For if $\limsup_{s\uparrow\infty} b(s) > \delta > 0$ then we can find a sequence $s_j \uparrow \infty$ so that $\|b(s_j)\| > \delta$ for $j \geq 1$. Without any loss of generality we may assume the sequence s_j is chosen so that the intervals

$$I_j = \left(s_j - \frac{\delta}{2K}, s_j + \frac{\delta}{2K}\right)$$

are disjoint. Then if $t \in I_j$ we have using (5)

$$\begin{aligned}\|b(t)\| &\geq \|b(s_j)\| - \|b(t) - b(s_j)\| \\ &\geq \delta - K|t - s_j| \geq \frac{\delta}{2}.\end{aligned}$$

This implies that $\int_{-\infty}^{\infty} \|b(s)\|^2 ds \geq \sum_j \int_{I_j} \|b(s)\|^2 ds = \infty$ which contradicts (4). From equation (1) we get

$$a_1(t) - a_1(0) = 2\int_0^t \|b(s)\|^2 ds$$

so $\lim_{t\to\infty} a_1(t) = \lambda$ exists and must be, in view of (i) an eigenvalue of A. Equation (3) implies

$$M(t) = M(0) = -2\int_0^t b(s)b^T(s)ds$$

and since $\|\int_0^\infty b(s)b^T(s)ds\| \leq \int_0^\infty \|b(s)\|^2 ds$ it follows that $\lim_{t\to\infty} M(t) = M_\infty$ exists. This proves part (ii) of the theorem. In order to prove that $\lambda = \lambda_n$ we note that the matrix of eigenvectors of $L(t)$ can be expressed as $U(t)U_0$ so that

$$f(t) = (U(t)U_0)^T e_1 = U_0^T U^T(t)e_1$$

and

$$\begin{aligned}
\frac{df}{dt} &= -U_0^T U^T(t)B(t)e_1 \\
&= U_0^T U^T(t)L(t)e_1 - a_1(t)U_0^T U^T(t)e_1 \\
&= U_0^T A U^T(t)e_1 - a_1(t)f(t) \\
&= \Lambda U_0^T U^T(t)e_1 - a_1(t)f(t) \\
&= \Lambda f(t) - a_1(t)f(t) \\
&= \Lambda f(t) - [f^T(t)\ \Lambda f(t)]f(t).
\end{aligned}$$

The solution of this equation, as can be verified directly, is

$$f(t) = \frac{e^{\Lambda t} f_0}{\|e^{\Lambda t} f_0\|}$$

and since $e_n^T f_0 \neq 0$ it follows that $\lim_{t\to\infty} f(t) = e_n$ and

$$\lim_{t\to\infty} a_1(t) = \lim_{t\to\infty} f^T(t)\ \ f(t) = \lambda_n.$$

<u>Remark</u>. The convergence proof above is adapted from Moser [2].

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