THE NUMERICAL APPROXIMATION OF THE EIGENVALUES AND EIGENVECTORS FOR SYMETRICAL MATRICES

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INTRODUCTION

One of the oldest ideas for the calculation of the eigenvalues and eigenvectors of the dense, symmetric matrices is Jacobi's algorithm introduced in 1845.

The procedure (computation method) focused specialists'attention as the parallel calculation thechniques were developing.

The paper presents Jacobi's rotation method and the corresponding program within the programming MATLAB medium for approximate calculation of eigenvalues and eigenvectors of the symmetric matrices.

1. JACOBI'S ROTATION METHOD

Let $\boldsymbol{A}$ be a square symmetric matrix of order n; then its eigenvalues are real and there exists an, orthonormal basis made of the eigenvectors $\boldsymbol{v_i}$, $\boldsymbol{i=\overline{1,n}}$ in which the equations $\boldsymbol{Av_i=\lambda_i v_i}$, $\boldsymbol{i=\overline{1,n}},$ hold and the matrix gets the diagonal form

$$\boldsymbol{D} = \begin{pmatrix} \lambda_1 & 0 & 0 \cdots 0 \\ 0 & \lambda_2 & 0 \cdots 0 \\ \cdots & \cdots & \cdots \\ 0 & 0 & 0 \cdots \lambda_n \end{pmatrix} \tag{1}$$

The basis can be chosen so as to lead to $\boldsymbol{\lambda_1 \geq \lambda_2 \geq \lambda_3 ... \geq \lambda_n}$.

If, moreover, matrix A is definitely positive, then $\boldsymbol{\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq ... \geq \lambda_n > 0}$ and

$$\lambda_1 = \|A\|_2 = \sup_{x \neq 0} \frac{\langle Ax, x\rangle}{\langle x, x\rangle}.$$

Lets $\boldsymbol{P}$ be the transformation matrix from the standard basis of the space $\boldsymbol{R^n}$ to the basis $(\boldsymbol{v_1, v_2, \ldots v_n})$. Once can easily see that $\boldsymbol{P^T P = I}$; hence $\boldsymbol{P}$ is orthogonal. If follows that $\boldsymbol{P^{-1} = P^T}$ and that $\boldsymbol{D = P^T A P}$.

In practice, the eigenvalues of matrix $\boldsymbol{A}$ cannot be actually identified by numerically solving the characteristic equation $\boldsymbol{det(A - \lambda I) = 0}$, because the roots of this polynomial are very "sensitive" to any modification in the coefficients of the polynomial.

The recommended method is to bring, by any possible means, the matrix to a diagonal form and then the eigenvalues can be wholly identified, since they are the elements on the main diagonal of $\boldsymbol{D}$.

Thus we aim , through similarity changes that do not modify the eigenvalues, to diminish, possibly up to the total vanishing, the non-diagonal elements of the matrix; thus we could eventually obtain the diagonal matrix.

Jacobi's method consists in performing a series of similarity transformations on the $\boldsymbol{A}$ matrix by using the simplest nontrivial orthogonal matrices (rotation matrices) of the form

$$\begin{array}{c} \qquad\quad p \qquad\qquad q \\ \boldsymbol{U} = \begin{pmatrix} 1 & 0 & 0 & . & 0 & & & & \\ 0 & 1 & 0 & & 0 & & & & \\ & & \ddots & & & & & & \\ 0 & \cdot & \cdot & \cos\varphi & \cdots & \sin\varphi & \cdot\cdot & 0 & \\ & \cdot & 1 & \cdot & & & & & \\ \vdots & \vdots & & \ddots & & \vdots & \vdots & & \\ 0 & \cdot & \cdot & -\sin\varphi & \cdots & \cos\varphi & \cdot & \cdot & 0 \\ & \cdot & \cdot & & \ddots & 1 & 0 & & \\ 0 & \cdots & \cdot & \cdot & & 0 & 1 & & \end{pmatrix}. \end{array} \tag{2}$$

The elements of matrix $\boldsymbol{U}$ are given by

$$\begin{cases} u_{ii} = 1 \text{ if } i \neq p \text{ and } i \neq q \\ u_{pp} = \cos\varphi,\ u_{pq} = \sin\varphi \\ u_{qp} = -\sin\varphi,\ u_{qq} = \cos\varphi \\ u_{ij} = 0 \text{ as remainder} \end{cases} . \quad (3)$$

The matrix U is orthogonal ($U^T U = I$ so $U^{-1} = U^T$) and, from a geometrical viewpoint, it represents a rotation of angle φ in the plane identified by the e_p and e_q directions.

We denote $A' = U^T A$ and $A'' = A' U = U^T A U$. In general, the elements of matrix A' are

$$\begin{cases} a'_{ij} = a_{ij} \text{ if } i \neq p \text{ and } j \neq q \\ a'_{pj} = a_{pj}.\cos\varphi - a_{qj}.\sin\varphi \\ a'_{qj} = a_{pj}.\sin\varphi + a_{qj}.\cos\varphi \end{cases} . \quad (4)$$

and the ones of matrix A'' are

$$\begin{cases} a''_{ij} = a'_{ij} \text{ if } i \neq p \text{ and } j \neq q \\ a''_{ip} = a'_{ip}.\cos\varphi - a'_{iq}.\sin\varphi \\ a''_{iq} = a'_{ip}.\sin\varphi + a'_{qj}.\cos\varphi \end{cases} . \quad (5)$$

If follows from (4) and (5) that

$$\begin{cases} a''_{pp} = a_{pp}\cos^2\varphi - 2a_{pq}\cos\varphi\sin\varphi + a_{qq}\sin^2\varphi \\ a''_{qq} = a_{pp}\sin^2\varphi + 2a_{pq}\cos\varphi\sin\varphi + a_{qq}\cos^2\varphi \\ a''_{pq} = (a_{pp} - a_{qq})\sin\varphi\cos\varphi + a_{pq}\cos 2\varphi \\ a''_{qp} = a''_{pq} \end{cases} . \quad (6)$$

We aim that largest (in absolute value) non-diagonal element, the should vanish, as a result of the rotation; we will choose the rows p and, so that a_{pq} will be the largest element (in absolute value) above the main diagonal and we shall state the condition that $a''_{pq} = 0$.

Taking into account (6) it follows that

$$\frac{1}{2}(a_{pq} - a_{qq})\sin 2\varphi + a_{pq}\cos 2\varphi = 0$$

and therefore

$$tg\, 2\varphi = \frac{2a_{pq}}{a_{qq} - a_{pp}}. \quad (7)$$

Hence, the angle of rotation is identified from (7). We will introduce the notations:

$$\theta = \frac{a_{qq} - a_{pp}}{2a_{pq}} \text{ and } tg\,\varphi = t \quad (8)$$

Since $tg2\varphi = \frac{2tg\varphi}{1 - tg^2\varphi}$, it results from (7) and (8) that $t^2 + 2\theta t - 1 = 0$.

By solving this equation we get

$$t_{1,2} = -\theta \pm \sqrt{\theta^2 + 1} = \frac{1}{\theta \pm \sqrt{\theta^2 + 1}}.$$

In order to avoid the case when, the denominator becomes very small we consider

$$t = \begin{cases} \dfrac{1}{\theta + sgn(\theta)\sqrt{\theta^2 + 1}} & \text{if } \theta \neq 0 \\ 1 & \text{if } \theta = 0 \end{cases} . \quad (9)$$

According to some elementary trigonometric formulas, we have:

$$\begin{cases} c = \cos\varphi = \dfrac{1}{\sqrt{1 + t^2}} \\ s = \sin\varphi = \dfrac{t}{\sqrt{1 + t^2}} \end{cases} . \quad (10)$$

From (9) and (10) it follows that $|t| \leq 1$,

$c \geq \frac{1}{\sqrt{2}}$, $|s| \leq \frac{1}{\sqrt{2}}$ and thus $\varphi \in \left[-\frac{\pi}{4}, \frac{\pi}{4}\right]$.

If we denote $S(C)$ the sum of the squares of the non-diagonal elements of any matrix C then , from (4) and (5), a direct calculation would lead us to:

$$S(A'') = S(A) - 2\ a_{pq}^2 + 2\,a_{pq}^{''2}.$$

Therefore, if we choose the angle of rotation φ according to (9) and (10), it results that $a''_{pq} = 0$ and thus

$$S(A'') = S(A) - 2\,a^2_{pq} \tag{11}$$

Since $a^2_{ij} \le a^2_{pq}$ *for* $i \ne j$, we get

$$S(A) \le n(n-1)\,a^2_{pq} \text{ or} \tag{12}$$

$$\frac{-2}{n(n-1)} S(A) \ge -2a^2_{pq}$$

We thus get, from (11) and (12),

$$S(A'') \le S(A)\left(1 - \frac{2}{n(n-1)}\right) \text{ for } n \ge 2 \tag{13}$$

Let us now consider a long series of rotations leading to the matrices $A_0, A_1, A_2, \ldots, A_k$ where $A_0=A$, $A_1=A''$, $A_2= A_1''$, etc

It follows from (13) that

$$S(A_k) \le \left(1 - \frac{2}{n(n-1)}\right)^k S(A) \tag{14}$$

But $1-\dfrac{2}{n(n-1)} \in (0,1)$ for $n > 2$, hence according to (14),

$$\lim_{k\to\infty} S(A_k) = 0$$

Thus, at the limit, the sequence $\{A_k\}$ tends tothe diagonal matrix. We can prove the theorem that follows. The matrix P is the result of product matrices $U_1, U_2, \ldots, U_k$.

Theorem [3]

Let us consider the eigenvalues λ_j of matrix A and let $a_{jj}^{(k)}$ be the diagonal elements of the matrix A_k. Then:

$$\left|a_{jj}^{(k)} - \lambda_j\right| \le \sqrt{S(A_k)}.$$

Since $a_{pq}^{(k)}$ is the largest (in absolute value) non-diagonal element of the A_k matrix, the following evaluation results:

$$S(A_k) \le (n^2 - n)\ (a_{pq}^{(k)})^2 < n^2\ \left(a_{pq}^{(k)}\right)^2.$$

From this theorem we obtain :

$$\left|a_{jj}^{(k)} - \lambda_j\right| < n\ \left|a_{pq}^{(k)}\right|. \tag{15}$$

The inequality (15) can be considered as a criterion for stopping the algorithm.

From inequality $n\ \left|a_{pq}^{(k)}\right| < eps.$, we will get the number k of the necessary rotations , to approximate the eigenvalues λ_j of the matrix A, with the diagonal elements $a_{ii}^{(k)}$ of matrix A_k.

The sequence of matrices A_k and P the transformation matrix, are recursively calculated by

$$\begin{cases} A_k = U_k^T A_{k-1} U_k,\ k \ge 1 \\ A_0 = A \end{cases}. \tag{16}$$

$$P := U_k P, \qquad k \ge 1 \tag{17}$$

The columns of the matrix P are the eigenvectors of matrix A.

2. THE COMPUTER PROGRAM

<u>Algorithm for the identification of eigenvalues through Jacobi's rotation procedure</u>

Introduce A, eps;

Repeat

Determine: $max:$ = the higest element in absolute value, above the main diagonal of matrix A;

(p,q): the position of this element;

Calculate $A := U^T * A * U$;

Calculate $P := U * P$;

Calculate $\boldsymbol{s:=}\left(\sum_{i=1}^{n}\sum_{\substack{j=1\\ i\neq j}}^{n} a_{ij}^{2}\right)^{\frac{1}{2}}$ until $s < eps$.

% Jacobi method for calculate eigenvalues and eigenvectors.
% We introduce ***A, s, n, eps, max1***.

```
m = 0;
P = eye (size(A));
while s > eps
for r = 1: n-1
for k = r+1 : n
if max1 < abs(A(r,k))
   max1 = abs(A(r,k));
    p = r;
    q = k;
     end
    end
 end
if A(p, q) = = 0
disp ('STOP')
break
   end
teta = (A(q,q) – A(p, p))/ 2 * A(p,q);
if teta = = 0
   t = 1;
   else
t = 1/ (teta + sign(teta)*(teta^2 +1)^(1/2));
end
c = 1 / (t^2+1)^(1/2);
s =  t / (t^2+1)^(1/2);
I = eye(size(A));
I(p,p) = c;
I(q,q) = c;
I(p,q) = s;
I(q,p) = -s;
disp ( 'the matrix U' )
disp ( I )
P = P * I ;
disp ( 'the matrix P' )
disp ( P )
A = I' * A * I;
disp (' the matrix A ')
disp ( A )
s = 0 ;
for r = 1 : n
for k = 1 :n
   if  r~ =k
   s = s + A(r,k)^2 ;
   end
  end
  end
 s = s^ (1/2)
 m =  m +1;
disp (' number iteration ')
disp (m)
  max1 = 0 ;
    end
%  The significance of the variables
%  A symmetric square matrix
%  n – the order of matrix A
%  max1 – contains the highest a(p,q) in absolute
%  value
%  eps – increased for s
%  P – the transformation matrix ; at the end, its
%  columns contain the eigenvectors of matrix A
%  At the end , on the main   diagonal of the matrix,
%one can read the eigenvalues of matrix A.
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Bibliography

1. Murgescu V. *Curs de analiza matematica si matematici speciale, vol. III, Rotaprint I. P. Iasi,1977.*

2. Paltineanu G., Matei P., Trandafir R. *Analiza numerica, Editura Conspress, Bucuresti, 1998.*

3. Schwarz H. E. *Numerical Analysis of Symmetric Matrices, Prentice-Hall, Inc. Englewood Cliffs, New Jersy, 1973.*

4. Agratini O., Coman Gh., Chiorean I., Trimbitas R. *Analiza numerica si teoria aproximarii, vol III, Presa Universitara, 1992.*

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