Diagonalisation of complex symmetric matrices using a modified Jacobi method

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The paper describes a method for the diagonalisation of complex symmetric matrices, using a sequence of plane rotations through complex angles, chosen so as to minimise the sum of the squares of the absolute values of the off-diagonal elements.

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Diagonalisation of complex symmetric matrices is required in the analysis of resonance structures in atomic collision cross sections (Gailitis, 1963; Trefftz, 1967). We describe a numerical method which has been found to be convenient.

Let A be a complex symmetric $N \times N$ matrix and let X be an orthogonal matrix; $\tilde{X}X = 1$ where $\tilde{X}$ is the transpose of X. Then $A' = \tilde{X}AX$ is symmetric and has the same eigenvalues as A. We seek a sequence of transformations, $A^{(1)} = \tilde{X}^{(1)}AX^{(1)}$, $A^{(n)} = \tilde{X}^{(n)}A^{(n-1)}X^{(n)}$, such that $A^{(n)}$ tends to a diagonal matrix as n increases. The eigenvalues of A are then given by the diagonal elements of $A^{(n)}$, in the limit of $n \to \infty$, and the eigenvectors are given by $T = X^{(1)}X^{(2)}X^{(3)} \ldots$.

It is necessary to specify a convergence criterion. Let $\Delta^{(n)}$ be the sum of the squares of the absolute values of the off-diagonal elements of $A^{(n)}$,

$$\Delta^{(n)} = \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} |A_{ij}^{(n)}|^2. \qquad (1)$$

The following criterion is adopted: given an accuracy parameter δ, the criterion is said to be satisfied if

$$\frac{\Delta^{(n)}}{N(N-1)} < \frac{\delta^2}{N(N+1)} \left\{ \sum_{i=1}^{N} \left| A_{ii} - \frac{1}{N}\sum_{j=1}^{N} A_{jj} \right|^2 + \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} |A_{ij}|^2 \right\}. \qquad (2)$$

It should be noted that the criterion is unaltered if a constant is added to all of the diagonal elements of A.

In the Jacobi method for the diagonalisation of a real symmetric matrix, the transformations are taken to be plane rotations. For a rotation through an angle $\theta/2$ in the (1, 2) plane, the elements of X are

$$\left.\begin{aligned} X_{11} &= X_{22} = \cos(\theta/2) \\ X_{12} &= -X_{21} = \sin(\theta/2) \\ X_{pq} &= \delta_{pq} \text{ for } p > 2 \text{ or } q > 2 \end{aligned}\right\} \qquad (3)$$

and the elements of $A' = \tilde{X}AX$ are

$$\left.\begin{aligned} A'_{12} &= A'_{21} = A_{12}\cos\theta + \tfrac{1}{2}(A_{11} - A_{22})\sin\theta \\ A'_{11} &= A_{11} - [\tfrac{1}{2}(A_{11} - A_{22})(1 - \cos\theta) + A_{12}\sin\theta] \\ A'_{22} &= A_{22} + [\tfrac{1}{2}(A_{11} - A_{22})(1 - \cos\theta) + A_{12}\sin\theta] \\ &\left.\begin{aligned} A'_{1p} &= A'_{p1} = A_{1p}\cos(\theta/2) - A_{2p}\sin(\theta/2) \\ A'_{2p} &= A'_{p2} = A_{2p}\cos(\theta/2) + A_{1p}\sin(\theta/2) \end{aligned}\right\} p > 2 \\ A'_{pq} &= A_{pq} \text{ for } p > 2 \text{ and } q > 2. \end{aligned}\right\} \qquad (4)$$

It follows that

$$A'^2_{1p} + A'^2_{2p} = A^2_{1p} + A^2_{2p}, \quad p > 2, \qquad (5)$$

and hence that the transformation leaves unchanged the sum of the squares of the off-diagonal elements other than A_{12}, A_{21}. For real symmetric matrices each rotation may be taken to be in the plane of the off-diagonal element largest in absolute value and the rotation angle may be chosen so as to reduce this element to zero; it may then be shown that the convergence criterion will be satisfied after a finite number of rotations (see, for example, Fröberg, 1965).

For complex symmetric matrices it is necessary to consider $\Delta^{(n)}$, the sum of the squares of the absolute values of the off-diagonal elements, in place of the sum of the squares. We therefore develop a modified method, which involves rotations through complex angles such that each rotation minimises $\Delta^{(n)}$. Let

$$D = |A_{12}|^2 + \sum_{p=3}^{N} \{|A_{1p}|^2 + |A_{2p}|^2\} \qquad (6)$$

be transformed to D' after a rotation in the (1, 2) plane. We then minimise Δ' on minimising D'. For rotation through an angle $\theta/2 = (u + iv)/2$ we obtain

$$D' = M\cosh(v + \gamma) + \frac{L}{2}\{\cosh[2(v + \beta)] - \cos[2(u + \alpha)]\} \qquad (7)$$

where

$$\left.\begin{aligned} M &= (S^2 - T^2)^{1/2}, \ \gamma = \ln[(S + T)/M], \\ S &= D - |A_{12}|^2, \ T = S - \sum_{p=3}^{N} |A_{1p} + iA_{2p}|^2 \end{aligned}\right\} \qquad (8)$$

and

$$\left.\begin{aligned} L &= |P^2 + Q^2|, \ \beta = \tfrac{1}{2}\ln[|P - iQ|^2/L] \\ \sin(2\alpha) &= (PQ^* + P^*Q)/L, \\ \cos(2\alpha) &= (|P|^2 - |Q|^2)/L \\ P &= \tfrac{1}{2}(A_{11} - A_{22}), \ Q = A_{12}. \end{aligned}\right\} \qquad (9)$$

For the minimisation of D', the solution for u is $u = -\alpha$ and the solution for v is obtained on minimising

$$\frac{L}{2}\{\cosh[2(v + \beta)] - 1\} + M\cosh(v + \gamma), \qquad (10)$$

that is, on solving

$$L\sinh[2(v + \beta)] + M\sinh(v + \gamma) = 0. \qquad (11)$$

The solution for v lies in the range $-\beta \leqslant v \leqslant -\gamma$ if $\beta \geqslant \gamma$, and in the range $-\gamma \leqslant v \leqslant -\beta$ if $\beta \leqslant \gamma$. Starting with an initial estimate of $v_0 = -(\beta + \gamma)/2$,

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equation (11) is solved using the Newton–Raphson method.

It may be shown that, if $PQ^* = iT/2$, the minimum value of D' occurs for rotation through a zero angle, $\theta/2 = 0$. This could lead to a failure to converge if each rotation was taken to be in the plane of the off-diagonal element largest in absolute value. We therefore carry out rotations in the planes $(p, q) = (1, 2), (1, 3), \ldots (1, N), (2, 3), (2, 4), \ldots (2, N), \ldots (N-1, N)$, and continue until the convergence criterion is satisfied. We have not obtained a formal proof of convergence, but satisfactory results have been obtained for a number of test cases. A listing of the FORTRAN program used is available on request.

Difficulties may arise for matrices with degenerate eigenvalues. Consider $A = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$ with eigenvalues $\lambda = \{(a + c) \pm [(a - c)^2 + 4b^2]^{1/2}\}/2$. The eigenvalues are equal if $(a - c) = \pm 2ib$, and in this case rotation through an angle $\theta/2$ in the $(1, 2)$ plane gives $A'_{12} = b \exp(\pm i\theta)$. The rotation will reduce the matrix to diagonal form only if we take $\theta = \pm i \infty$. For matrices of this type a different method is required.

The method of the present paper is similar to a method used by Eberlein (1962) for the diagonalisation of arbitrary complex matrices. The methods differ in that Eberlein uses transformations which are not plane rotations, and in that her transformations give only an approximate minimisation of $\Delta^{(n)}$.

References

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FRÖBERG, C.-E. (1965). *Introduction* to *Numerical Analysis*, p. 110. London: Addison-Wesley Publishing Co.

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Book Review

Systems and Computer Science, edited by J. F. Hart and S. Takasu, 1968; 249 pages. (*Toronto University Press, Oxford University Press*, 166s. 6d.)

This book contains revised and extended versions of ten papers given at a two-day conference on Systems and Computer Science at the University of Western Ontario in September 1965. The purpose of the conference was to stimulate teaching and research by drawing attention to relevant theoretical topics, automata, theorem proving, linguistics and general systems.

'In line with these objectives the invited lecturers were asked to bring out the nature of the different fields, the current problems and an opinion concerning the hope for the future.' The contents are

- On the Structure of Finite Automata, J. Hartmanis
- Synthesis of Sequential Machines, J. A. Brzozowski
- Techniques for Manipulating Regular Expansions, Robert McNaughton
- Some Comments on Self-Reproducing Automata, Michael A. Arbib
- Multiple Control Computer Models, C. C. Elgot, A. Robinson, and J. D. Rutledge
- Explicit Definitions and Linguistic Dominoes, S. Gorn
- Heuristic and Complete Processes in the Mechanisation of Theorem Proving, J. A. Robinson
- An Approach to Heuristic Problem Solving and Theorem Proving in the Propositional Calculus, S. Amarel
- New Directions in General Theory of Systems, M. D. Mesarovič
- Concerning an Algebraic Theory of Systems, T. G. Windeknecht.

Most of the papers are short (less than twenty pages), surveying recent work and/or discussing research problems. In the list above the first four, last two and the paper by Robinson come in this group. They all fulfil the brief given; if particular mention is made of the stimulating paper by Arbib, not least for the battery of problems he discusses, this is in no way to denigrate the others. These papers provide numerous references, some as late as 1967, to more detailed treatments of the work discussed.

Elgot *et al.* report a specific piece of research—an attempt at defining a formal model of a multiple processor system. It is shown that use of parallelism in computing functions involving composition is within the scope of the model and the extension to recursive functions should be possible.

Amarel's paper, being nearly 100 pages, must represent a considerable extension of the material actually used at the conference. It discusses in detail the evolution of three sets of procedures of increasing efficiency for finding minimal (in the sense defined) proofs of theorems in the propositional calculus. It illustrates the relation between efficiency and convenient representations of the problem's solution space, and like Robinson's paper exemplifies heuristics which are subsequently shown to preserve completeness. The difficult problems of mechanising the evolutionary steps between the sets of procedures are discussed.

Gorn's paper is concerned with the problem of translation between different languages which, starting from a common ancestor, arise by having different sets of explicit definitions introduced and used in succeeding generations. A large part of the paper is devoted to the explicit definitions which make Professor Gorn's current language differ from that of his audience. The reviewer has not yet completed a translation.

The book is nicely produced, but at this price even librarians must wince.

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