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Applied Mathematical Modelling

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Numerical determination for solving the symmetric eigenvector problem using genetic algorithm



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ARTICLE INFO

Article history: Received 5 January 2015 Revised 11 November 2015 Accepted 4 December 2015 Available online 18 December 2015

Keywords:
Eigenvector
Eigenvalue
Genetic algorithm
Symmetric matrices
Hermitian matrices
Computational methods

ABSTRACT

The eigenvalues and eigenvectors of a matrix have many applications in engineering and science. For example they are important in studying and solving structural problems, in the treatment of signal or image processing, in the study of quantum mechanics and in certain physical problems. It is therefore essential to analyze methodologies to obtain the eigenvectors and eigenvalues of symmetric and Hermitian matrices. In this paper the authors present a methodology for obtaining the eigenvectors and eigenvalues of a symmetric or Hermitian matrix using a genetic algorithm. Unlike other methodologies, the process is centred in searching the eigenvectors and calculating the eigenvalues afterwards. In the search of the eigenvectors a genetic-based algorithm is used. Genetic algorithms are indicated when the search space is extended, unknown or with an intricate geometry. Also, the target vector space can be either real or complex, allowing in this way a wider field of application for the proposed method. The algorithm is tested comparing the results with those obtained by other methods or with the values previously known. So, seven applications are included: a real symmetric matrix corresponding to a vibrating system, a complex Hermitian matrix and an important application of the diagonalization problem (Coope matrix) corresponding to quantum mechanics examples, a physical problem in which data are analysed to reduce the number of variables, a comparison with the power method and the studies of a degenerate and an ill-conditioned matrix.

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1. Introduction

The problem of determining the set of eigenvectors and eigenvalues of a matrix is known as the complete eigenvalue problem. This matter is presented in several problems, as solving differential equations, studying the stability and behaviour of mechanical structures and determining the allowed states of quantum systems.

Given a matrix a, A, representing a linear transformation on a vector space V(K) defined over a field K, the problem results in the determination of the vectors, eigenvectors u, and scalars, eigenvalues A, that solve the equation:

$$A \cdot u = \lambda u. \tag{1.1}$$

A classic approach is to calculate the eigenvalues as the solution of:

$$\det\left(A - \lambda \cdot I\right) = 0. \tag{1.2}$$

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That is, solving a polynomial equation (characteristic polynomial) $P(\lambda) = 0$. Once the eigenvalues are known, the eigenvector corresponding to each eigenvalue λ_i is calculated solving the linear system:

$$(A - \lambda_i \cdot I) \cdot u^{(i)} = 0. \tag{1.3}$$

Leverrier and Krylov methods can be used to solve the characteristic polynomial [1–4]. However, the calculation of the numeric solution has instability problems because of the dependence of the zeroes estimation from the polynomial coefficients. Moreover, there are numerical methods for diagonalizing a symmetric matrix (Parlettt,1981, [5]; Wilkinson,1965 [6]; Cullun, 1985 [7]). Sometimes not all the eigenvalues are calculated, limiting the efforts to some of them.

The eigenvalue problem can also be converted in an optimization problem, where an adequate function can be minimized or maximized computing its gradient and hessian, and obtaining the eigenvectors of the matrix. In this case the non-deterministic and stochastic methods can be of interest. These methods, that have been applied in physics, economy and other fields, can be found in several papers (Kirkpatrick, 1983 [8]; Van Laarhoven, 1987 [9]; Goldberg, 1989 [10]).

Some authors (Subhajit, 2011 [11]) have used genetic algorithms to calculate some of the eigenvalues by means of the Rayleigh quotient.

Other methods that don't need to solve the characteristic polynomial are the power method and its variants, (Demidovich, 1993 [3]; Volkov, 1987 [4]). Let the eigenvalues λ_1 , λ_2 , ..., λ_n ordered by their magnitudes,

$$|\lambda_1| \ge |\lambda_2| \ge \dots \ge |\lambda_n|. \tag{1.4}$$

When considering the repeated action of the matrix over an arbitrary vector (expressed using the eigenvectors basis):

$$A \cdot y = A \cdot (y^{1} \cdot u_{1} + y^{2} \cdot u_{2} + ... + y^{n} \cdot u_{n}) = y^{1} \cdot \lambda \cdot u_{1} + y^{2} \cdot \lambda_{2} \cdot u_{2} + ... + y^{n} \cdot \lambda_{n} \cdot u_{n}, \tag{1.5}$$

$$A^{N} \cdot y = \lambda_{1}^{N} \cdot \left[y^{1} \cdot u_{1} + y^{2} \cdot \left(\frac{\lambda_{2}}{\lambda_{1}} \right)^{N} \cdot u_{2} + \dots + y^{n} \cdot \left(\frac{\lambda_{n}}{\lambda_{1}} \right)^{N} \cdot u_{n} \right]. \tag{1.6}$$

The convergence to the first eigenvector depends on the relation(λ_2/λ_1). There are variations of the method to accelerate the convergence velocity: the shifted power method, Aitken's method, (Demidovich, 1993 [3]; Volkov, 1987 [4]), or the Jacobi method and others if the matrix is symmetric. When the first eigenvector is calculated, a process of deflation removes it from the search space.

Other possibility that can be used is the QR method that makes orthogonal transforms according to the spectral theorem for symmetric matrices (Golub, G.H,1996 [12]; Endre Süli,2003 [13]). So, the QR decomposition method factors any matrix A as A = QR, where Q is an orthogonal matrix and R is a non-singular upper matrix. This is the base of the QR eigenvalue algorithm used for symmetric and Hermitian matrices. A variation of this method, known as Shifted QR makes a previous modification of the matrix A, $A - \alpha I = QR$ to speed up the convergence of the algorithm.

2. Numeric methodology

In the present paper an implementation of a genetic algorithm is presented for calculating the first eigenvector and eigenvalue of a symmetric or Hermitian matrix. To determine the rest of eigenvectors, the matrix is modified by a rotation that transforms the first vector of the canonical basis into the calculated eigenvector. The eigenvectors of the transformed matrix have the first component equal to zero.

Once all the eigenvectors have been calculated, the change of basis can be inverted, obtaining the components of the eigenvectors in the canonical basis.

2.1. Search of the first eigenvector

Given a matrix A, obtaining the eigenvectors is equivalent to solve the equation:

$$A \cdot u_i = \lambda_i \cdot u_i$$
. (2.1)

For simplicity, it can be assumed the normalized eigenvectors, $||u_i|| = 1$. Vectors u_i and its images $z = A \cdot u_i$ are collinear, and so that it meets:

$$u_i^T \cdot z = u_i^T \cdot A \cdot u_i = \lambda_i \cdot u_i^T \cdot u_i = \lambda_i \cdot ||u_i||^2 = \lambda_i. \tag{2.2}$$

Given any vector of module 1 close to the eigenvector $x = u_i + e$, the image can be decomposed into two parts one collinear and one perpendicular:

$$\begin{split} z &= A \cdot x = A \cdot (u_i + e) = \lambda_i \cdot u_i + A \cdot e = \lambda_i \cdot [x - e] + A \cdot e = \lambda_i \cdot x + [A - \lambda_i \cdot I] \cdot e \\ &= \lambda_i \cdot x + \varepsilon \cdot x + z_\perp = (\lambda_i + \varepsilon) \cdot x + z_\perp. \end{split}$$

So, if the vectors are normalized, ||u|| = 1 any unitary vector close to the eigenvector, $x = u_i + e$ has an image which has parallel and orthogonal components:

$$z = A \cdot x = (\lambda_i + \varepsilon) \cdot x + z_{\perp}. \tag{2.3}$$

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