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Review

Eigenproblem Basics and Algorithms

Lorentz Jäntschi

Department of Physics and Chemistry, Technical University of Cluj-Napoca, Muncii 103-105, 400641 Cluj-Napoca, Romania; lorentz.jantschi@ubbcluj.ro; Tel.: +40-264-401775

Abstract: Some might say that the *eigenproblem* is one of the examples people discovered by looking at the sky and wondering. Even though it was formulated to explain the movement of the planets, today it has become the *ansatz* of solving many linear and nonlinear problems. Formulation in the terms of the eigenproblem is one of the key tools to solve complex problems, especially in the area of molecular geometry. However, the basic concept is difficult without proper preparation. A review paper covering basic concepts and algorithms is very useful. This review covers the basics of the topic. Definitions are provided for defective, Hermitian, Hessenberg, modal, singular, spectral, symmetric, skew-symmetric, skew-Hermitian, triangular, and Wishart matrices. Then, concepts of characteristic polynomial, eigendecomposition, eigenpair, eigenproblem, eigenspace, eigenvalue, and eigenvector are subsequently introduced. Faddeev–LeVerrier, von Mises, Gauss–Jordan, Pohlhausen, Lanczos–Arnoldi, Rayleigh–Ritz, Jacobi–Davidson, and Gauss–Seidel fundamental algorithms are given, while others (Francis–Kublanovskaya, Gram–Schmidt, Householder, Givens, Broyden–Fletcher–Goldfarb–Shanno, Davidon–Fletcher–Powell, and Saad–Schultz) are merely discussed. The eigenproblem has thus found its use in many topics. The applications discussed include solving Bessel's, Helmholtz's, Laplace's, Legendre's, Poisson's, and Schrödinger's equations. The algorithm extracting the first principal component is also provided.

Keywords: algorithms; characteristic polynomial; eigendecomposition; eigenfunction; eigenpair; eigenproblem; eigenspace; eigenvalue; eigenvector; PCA (principal component analysis); PCR (principal component regression)

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1. Introduction

About 250 years ago, the study of the motion of rigid bodies, with direct interest to the movement of the planets, led to the first formulation of the eigenproblem. In general, the eigenproblem is about minimization of the maximum eigenvalue of an matrix that depends affinely on a variable, subject to some constraint. Euler [1], Lagrange [2], Laplace [3], Fourier [4], and Cauchy [5] studied the problem.

Linear algebra was introduced through systems of linear equations. The terms matrix, determinant, and minor, as are used today, were introduced by Sylvester around the year 1850 [6].

Symmetry plays an essential role. Symmetric real-valued matrices have real eigenvalues. Hermite [7] extended this result to complex valued matrices mirroring the conjugate transpose (Hermitian matrices), and Sylvester [8] to Hessians (Hessian matrices).

Some authors [9] noted "any attempt to write a complete overview on the research on computational aspects of the eigenvalue problem a hopeless task". Here, no such thing is claimed, and instead for the eigenproblem is provided a bottom-up approach, from simple to complex on the one hand and from old to new on the other hand. The style used in specifying the algorithms was previously used in [10].

As mentioned before, the characteristic polynomial and the eigenproblem appeared for the first time in the context of solving complex problems in physics, but the area of

their use has been expanded since, and today covers a diverse set of applications. Even if, in most instances, the problems involve operating on real-valued data ($\mathbb{R}$), in some cases, the mathematical and numerical treatise has proved to be more convenient in the complex domain ($\mathbb{C}$), and the literature on calling for eigenproblem and characteristic polynomial formulations and solutions is expanding and growing. Since a real number can always be seen as a particular case of a complex number, a number can be seen as a particular case of an 1-tuple (or a vector with one component), or a matrix with only one entry. Thus, since the eigenproblem is formulated and uses all these fields (a field is generally a set of elements having defined multiplication and addition operations analogous to multiplication and addition in the real number system), the tendency to generalize is perfectly justified, so $\mathbb{K}$ will be referred to the field generalizing those alternatives.

Generally, a matrix is an ordered set of values. Formally, a matrix is a two-dimensional arrangement of its values. Sylvester [6] appears to be the first to use the arrangement of the matrix elements in rows and columns. A square matrix has an equal number of columns and rows. Thus, if $A = (a_{i,j}) \in \mathbb{K}^{n\times n}$ (in general $m \neq n$) is a square matrix, then $a_{i,j} \in \mathbb{K}$ are the elements of the matrix for each $i = 1, \ldots, n$ and $j = 1, \ldots, n$ (integers). On the field ($\mathbb{K}$), one can recognize the existence of the addition ($C = A + B$, defined as $c_{i,j} = a_{i,j} + b_{i,j}$ for all $1 \leq i, j \leq n$), and that of the multiplication ($C = A \times B$, defined as $c_{i,j} = \sum_{k=1}^{n} a_{i,k} \times b_{k,j}$ for all $1 \leq i, j \leq n$). A second multiplication operation ($C = \alpha \times A$, defined as $c_{i,j} = \alpha \times a_{i,j}$ for any $\alpha \in \mathbb{K}$ and all $1 \leq i, j \leq n$) provides a linear space. One immediate consequence is the existence of the subtraction ($C = A - B$, defined as $c_{i,j} = a_{i,j} - b_{i,j}$ for all $1 \leq i, j \leq n$).

Two particular matrices are of importance: the zero valued ($O = (\omega_{i,j}) \in \mathbb{K}^{n\times n}, \omega_{i,j} = 0$ for all $1 \leq i, j \leq n$), and the identity matrix ($I = (\iota_{i,j}) \in \mathbb{K}^{n\times n}, \iota_{i,j} = \delta_{i,j}$ for all $1 \leq i, j \leq n$ and $\delta_{i,j}$ is the Kronecker delta [11]).

Two matrix operations are also of importance: the transpose ($C = A^T$, defined as $c_{i,j} = a_{j,i}$ for all $1 \leq i, j \leq n$), and the conjugate ($C = \overline{A}$, defined as $c_{i,j} = \overline{a_{i,j}}$ for all $1 \leq i, j \leq n$).

2. Basic Concepts

Definition 1. *Characteristic polynomial.*

The characteristic polynomial P (in λ) associated with $A \in \mathbb{K}^{n\times n}$ is:

$$P(\lambda, A) \leftarrow |\lambda \times I - A| \tag{1}$$

where $|\cdot|$ (symbolically) evaluates the determinant. The characteristic polynomial is always a monic polynomial (leading coefficient is 1) of degree n.

Definition 2. *Eigenvalue.*

An eigenvalue (of A) is a root of the characteristic equation:

$$\lambda \text{ eigenvalue of } A \iff |\lambda \times I - A| = 0 \tag{2}$$

Equation (2) always has n roots, even if some of them may not be distinct, but multiple. Equation (2) provides all eigenvalues of A.

Definition 3. *Eigenproblem.*

The eigenproblem is:

$$\text{For } A \in \mathbb{K}^{n\times n} \text{ determine } \lambda \in \mathbb{K} \text{ and } v \in \mathbb{K}^n, v \neq 0, \text{ s.t. } A \times v = \lambda \times v \tag{3}$$

In Equation (3), λ is an eigenvalue and v is an *eigenvector* of A, while the (λ, v) pair is an *eigenpair* of A. One should notice that Equation (2) provides a direct method for calculation of the eigenvalues, which, when inserted in Equation (3), provides their

associated eigenvectors. The set $\{v : (\lambda \times I - A)v = 0\}$ is the *eigenspace* of A associated with λ being the union of the zero vector with the set of all eigenvectors of A associated with λ (nullspace of $\lambda \times I - A$). Furthermore, any nonzero scalar multiple of an eigenvector is also an eigenvector, so *unit eigenvectors* may be provided when convenient.

The eigenproblem is generalized when another matrix, B ($B \in \mathbb{K}^{n \times n}$), is inserted in Equation (3): $A \times v = \lambda \times B \times v$.

Example 1. $\mathbb{K} = \mathbb{C}$.

Let us consider two complex valued matrices with a certain similarity in their structure (Table 1, $i \leftarrow \sqrt{-1}$).

Table 1. Eigenproblem of two complex matrices containing the roots of $y^4 = 1$.

A	1	2	3	4
1	1	i	-1	$-i$
2	i	-1	$-i$	1
3	-1	$-i$	1	i
4	$-i$	1	i	-1
$P(\lambda, A) = \lambda^4$; eigenvector of $\lambda = -2$: $\begin{bmatrix} \mathrm{i} & -1 & -\mathrm{i} & 1 \end{bmatrix}^{\mathrm{T}}$				
B	1	2	3	4
1	-1	1	i	$-i$
2	$-i$	i	-1	1
3	1	-1	$-i$	i
4	i	$-i$	1	-1
$P(\lambda, B) = (\lambda + 2)\lambda^3$; eigenvector of $\lambda = 0$: $\begin{bmatrix} -\mathrm{i} & 1 & 0 & 0 \end{bmatrix}^{\mathrm{T}}$; eigenvector of $\lambda = 0$: $\begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}^{\mathrm{T}}$				

One should notice that matrix A contains the same elements as matrix B, but with an increased symmetry, a property that is transferred to the eigenspace, since the eigenvector of matrix A is the dot product of the eigenvectors of matrix B. More about real eigenvalues of complex valued matrices can be found in [12] regarding their applications in signal processing [13].

Example 2. *Molecular topology.*

A chemical compound—namely 1,4,2,5-diazadiborine—compound 8 in [14] was geometrically represented [14,15], and the topological distance matrix was calculated on the heavy atoms skeleton ([Di] in Figure 5 from [15]). Here, the topological distance matrix (Table 2) is used to exemplify the eigenproblem on $\mathbb{K} = \mathbb{R}$.

Table 2. Eigenproblem of a symmetrical matrix from $\mathbb{R}^{6 \times 6}$.

A	1	2	3	4	5	6
1	0	1	2	3	2	1
2	1	0	1	2	3	2
3	2	1	0	1	2	3
4	3	2	1	0	1	2
5	2	3	2	1	0	1
6	1	2	3	2	1	0
Eigenvalue	Eigenvector					
-4	$\begin{bmatrix} -1 & -1 & 0 & 1 & 1 & 0 \end{bmatrix}^{\mathrm{T}}$					
-1	$\begin{bmatrix} -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}^{\mathrm{T}}$					
0	$\begin{bmatrix} -1 & 1 & 0 & -1 & 1 & 0 \end{bmatrix}^{\mathrm{T}}$					
9	$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}^{\mathrm{T}}$					

The characteristic polynomial of the matrix A from Table 2 is: $P(\lambda, A) = (\lambda+4)^2(\lambda+1)\lambda^2(\lambda-9)$. One should notice that there are only four distinct eigenvalues here (-4, -1, 0, and 9), so there are only four distinct unit eigenvectors as well. A (square) matrix is *diagonal* if the entries outside the main diagonal are all zero (with z as an arbitrary value):

$$A \in \mathbb{K}^{n\times n} \text{ diagonal} \iff a_{i,j} = \begin{cases} 0 & \text{if } i \neq j \\ z \in \mathbb{K} & \text{otherwise} \end{cases} \tag{4}$$

A square matrix is *invertible* if its inverse exists ($B = A^{-1}$ in Equation (5)):

$$A \in \mathbb{K}^{n\times n} \text{ invertible} \iff \exists B \in \mathbb{K}^{n\times n} \text{ s.t. } A\times B = I = B\times A \tag{5}$$

A square matrix is *diagonalizable* if a diagonal form is obtainable:

$$A \in \mathbb{K}^{n\times n} \text{ diagonalizable} \iff \exists B \in \mathbb{K}^{n\times n} \text{ invertible s.t. } B^{-1}\times A\times B \text{ diagonal} \tag{6}$$

If $D \leftarrow B^{-1}\times A\times B$ from Equation (6), then $B\times D\times B^{-1}$ is the *eigendecomposition* of A ($A = B\times D\times B^{-1}$).

If $A \in \mathbb{K}^{n\times n}$ has n distinct eigenvalues (λ_i, $i = 1, \ldots, n$), then it has n linearly independent eigenvectors (v_i, $i = 1, \ldots, n$). M, constructed from its eigenvectors as columns (${M^T}_i \leftarrow v_i$), is the *modal matrix*(of A), and $M^{-1}\times A\times M$ is the *spectral matrix*(of A) and is a diagonal matrix with the eigenvalues of A on the main diagonal [16] (and $M^{-1} = M^H$).

On the contrary, a *defective matrix* is a square matrix that does not have a complete basis of eigenvectors, and is therefore not diagonalizable.

3. Algorithms

Algorithm 1 shows the characteristic polynomial coefficients and roots.

Given a matrix, A, the coefficients of the characteristic polynomial (Equation (1)) can be easily provided by an algorithm that was first suggested by LeVerrier [17]. One good alternative to provide the roots of the characteristic polynomial when all its coefficients are real is [18]. Other recently reported alternatives for finding roots include [19,20].

Algorithm 1 Faddeev–LeVerrier

Input: A //square matrix
  function FADDEEV(&A)
    // TRACE, UNITM, MULTC, ADDM, MULTM defined in Appendix A
    $n \leftarrow$ COUNT(A); $B \leftarrow A$; $c \leftarrow []$; $c[0] \leftarrow 1$
    For($i \leftarrow 1$; $i \leq n$; $i \leftarrow i+1$)
      $c[k] \leftarrow -$TRACE(B)$/i$; $D \leftarrow$ UNITM(n); $D \leftarrow$ MULTC($c[k], D$)
      $B \leftarrow$ ADDM(B, D); $B \leftarrow$ MULTM(A, B)
    EndFor
    RETURN(c) // $c \leftarrow ChP(A)$
  end function
  $c \leftarrow$ FADDEEV(A) // c is the characteristic polynomial of A
Output: c // c is the characteristic polynomial of A

Algorithm 2 shows the von Mises iteration.

Given a diagonalizable matrix, A, the von Mises iteration [21] will produce a nonzero vector, v, and a corresponding eigenvector of λ_1 and A, that is, $Av = \lambda_1 v$, where λ_1 is the greatest (in absolute value) eigenvalue of A.

The von Mises iteration starts with an approximation to the dominant eigenvector or a random vector, v_0, and uses the recurrence relation (7) ($k = 0, 1, \ldots$).

$$v_{k+1} \leftarrow \frac{A \times v_k}{\|A \times v_k\|} \tag{7}$$

Let us consider the Example 2 eigenproblem, in which the greatest eigenvalue is 9 and its associated eigenvector is $\begin{bmatrix}1 & 1 & 1 & 1 & 1 & 1\end{bmatrix}^T$. Table 3 lists a series of case studies regarding the convergence of Algorithm 1.

Table 3. Case studies of Algorithm 2 convergence for the Example 2 eigenproblem.

Case	Initial Eigenvector	Iterations	Note
1	$\begin{bmatrix}1 & 1 & 1 & 1 & 1 & 1\end{bmatrix}^{\mathrm{T}}$	1	Iterations is the number of Equation (7) iterations to acquire an residual error less than 5×10^{-5} for each component of the final eigenvector (each is then approximately 1.0000). Final eigenvector: $\begin{bmatrix}1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000\end{bmatrix}^{\mathrm{T}}$.
2	$\begin{bmatrix}0 & 1 & 1 & 1 & 1 & 1\end{bmatrix}^{\mathrm{T}}$	12	
3	$\begin{bmatrix}0 & 0 & 1 & 1 & 1 & 1\end{bmatrix}^{\mathrm{T}}$	13	
4	$\begin{bmatrix}0 & 0 & 0 & 1 & 1 & 1\end{bmatrix}^{\mathrm{T}}$	14	
5	$\begin{bmatrix}0 & 0 & 0 & 0 & 1 & 1\end{bmatrix}^{\mathrm{T}}$	14	
6	$\begin{bmatrix}0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}^{\mathrm{T}}$	14	

The algorithm implementing von Mises iteration is given as Algorithm 2.

Algorithm 2 Principal eigenvector

Input: A //diagonalizable matrix
  procedure PRINCIPAL(&A, &v)
    $M\_Eps \leftarrow 10^{-7}$
    For(; ;)
      $w \leftarrow$ MULTM(A, v); $w \leftarrow$ UNITV(w)
      If(DIFFV(v, w)<M_Eps) BREAK Else $v \leftarrow w$ EndIf
    EndFor
    $v \leftarrow w$
  end procedure
  $n \leftarrow$ COUNT(A); $v \leftarrow$ INITV($n, 1$) // $v \leftarrow 1$; INITV($n, -1$) for $v \leftarrow$ RAND
  PRINCIPAL(A, v) // v is the principal eigenvector of A
Output: v // v is the principal eigenvector of A

If λ_1 is strictly greater in magnitude than other eigenvalues of A, and the starting vector, v_0, has a nonzero component in the direction of an eigenvector associated with λ_1, then v_k converges to an eigenvector associated with λ_1. Without the two assumptions above, v_k does not necessarily converge. The convergence is geometric, with the ratio $|\lambda_2/\lambda_1|$, where λ_2 denotes the second dominant eigenvalue. The convergence is slow if λ_2 is close in magnitude to λ_1.

Algorithm 3 shows the Gauss–Jordan elimination.

Given a diagonalizable matrix, A, and an eigenvalue, λ, the Gauss–Jordan elimination [22] is able to provide the diagonalized matrix, a basis to derive a nonzero eigenvector, v. It is given as Algorithm 3.

Consider again the Example 2 eigenproblem, in which the goal now is to obtain the eigenvectors associated with the eigenvalues.

It should be noticed that $C \times v = 0$ from Table 4 has one degree of freedom (diagonalization produced a zero on the main diagonal of matrix C in Table 4, v_6 in $C \times v$), therefore any arbitrary value ($v_6 \neq 0$, since it must be $v \neq 0$) of its associated variables will provide an eigenvalue. For instance, $v_6 \leftarrow 1$ will provide the same solution as the one listed in Table 2 ($v_6 = v_5 = v_4 = v_3 = v_2 = v_1 = 1$). Additionally, while $C \times v = 0$ has one degree of freedom by necessity, $\lambda = 9$ has a multiplicity of 1 in $|\lambda \times I - A| = 0$ (indeed, see Example 2).

Algorithm 3 Matrix diagonalization

Input: A //a square diagonalizable matrix

procedure GAUSSJ(&A, &B, &C)
$n \leftarrow$ COUNT(A); $M\_Eps \leftarrow 10^{-7}$
For($i \leftarrow 0; i < n; i \leftarrow i+1$)
$k \leftarrow i$
For($j \leftarrow i+1; j < n; j \leftarrow j+1$) If($|a[j][i]| > |a[k][i]|$) $k \leftarrow j$ EndIf EndFor
If($|a[i][k]| < M\_Eps$) CONTINUE EndIf
If($k \neq i$)
$x \leftarrow c[k]; c[k] \leftarrow c[i]; c[i] \leftarrow x$
For($j \leftarrow 0; j < n; j \leftarrow j+1$) $x \leftarrow b[k][j]; b[k][j] \leftarrow b[i][j]; b[i][j] \leftarrow x$ EndFor
For($j \leftarrow 0; j < n; j \leftarrow j+1$) $x \leftarrow a[k][j]; a[k][j] \leftarrow a[i][j]; a[i][j] \leftarrow x$ EndFor
EndIf
$x \leftarrow a[i][i]; c[i] \leftarrow c[i]/x$
For($j \leftarrow 0; j < n; j \leftarrow j+1$) $b[i][j] \leftarrow b[i][j]/x; a[i][j] \leftarrow a[i][j]/x$ EndFor
For($j \leftarrow 0; j < n; j \leftarrow j+1$) If($i \neq j$)
$x \leftarrow a[j][i]; c[j] \leftarrow c[j] - x \cdot c[i]$
For($k \leftarrow 0; i < n; k \leftarrow k+1$) $b[j][k] \leftarrow b[j][k] - x \cdot b[i][k]$ EndFor
For($k \leftarrow 0; i < n; k \leftarrow k+1$) $a[j][k] \leftarrow a[j][k] - x \cdot a[i][k]$ EndFor
EndIf EndFor
end procedure
GAUSSJ(A, B, C) // square matrix A is diagonalized here

Output: A // $A \leftarrow$ diagonalized A, $B \leftarrow A^{-1}$ if exists, $C \leftarrow A^{-1}C$ if exists

$C \times v = 0$ from Table 5 has two degrees of freedom (diagonalization produced two zeroes on the main diagonal of matrix C in Table 5, v_5 and v_6 in $C \times v$), so any arbitrary value ($v_5 \cdot v_6 \neq 0$, since it must be $v \neq 0$) of its associated variable will provide an eigenvalue. For instance, $v_5 \leftarrow 1$ and $v_6 \leftarrow 0$ will provide the same solution as the one listed in Table 2 ($v_6 = v_3 = 0$, $v_5 = v_4 = 1$, $v_2 = v_1 = -1$). Furthermore, while $C \times v = 0$ has two degrees of freedom by necessity, $\lambda = -4$ has a multiplicity of 2 in $|\lambda \times I - A| = 0$ (indeed, see Example 2).

Table 4. Diagonalization of $9 \cdot I - A$ (Table 2, Example 2).

B	1	2	3	4	5	6	C	1	2	3	4	5	6
1	9	−1	−2	−3	−2	−1	1	1	0	0	0	0	−1
2	−1	9	−1	−2	−3	−2	2	0	1	0	0	0	−1
3	−2	−1	9	−1	−2	−3	3	0	0	1	0	0	−1
4	−3	−2	−1	9	−1	−2	4	0	0	0	1	0	−1
5	−2	−3	−2	−1	9	−1	5	0	0	0	0	1	−1
6	−1	−2	−3	−2	−1	9	6	0	0	0	0	0	0

$$C \times \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{bmatrix} = \begin{bmatrix} v_1 - v_6 \\ v_2 - v_6 \\ v_3 - v_6 \\ v_4 - v_6 \\ v_5 - v_6 \\ 0 \end{bmatrix}$$

$B \leftarrow 9 \cdot I - A$; C from Algorithm 3 on B.

Table 5. Diagonalization of $-4 \cdot I - A$ (Table 2, Example 2).

B	1	2	3	4	5	6	C	1	2	3	4	5	6
1	−4	−1	−2	−3	−2	−1	1	1	0	0	0	1	−1
2	−1	−4	−1	−2	−3	−2	2	0	1	0	0	1	0
3	−2	−1	−4	−1	−2	−3	3	0	0	1	0	0	1
4	−3	−2	−1	−4	−1	−2	4	0	0	0	1	−1	1
5	−2	−3	−2	−1	−4	−1	5	0	0	0	0	0	0
6	−1	−2	−3	−2	−1	−4	6	0	0	0	0	0	0

$$C \times \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{bmatrix} = \begin{bmatrix} v_1 + v_5 - v_6 \\ v_2 + v_5 \\ v_3 + v_6 \\ v_4 - v_5 + v_6 \\ 0 \\ 0 \end{bmatrix}$$

$B \leftarrow -4 \cdot I - A$; C from Algorithm 3 on B.

$C \times v = 0$ from Table 6 has one degree of freedom (diagonalization produced one zero on the main diagonal of matrix C in Table 6, v_6 in $C \times v$), so any arbitrary value ($v_6 \neq 0$, since it must be $v \neq 0$) of its associated variable will provide an eigenvalue. For instance, $v_6 \leftarrow zzz$ will provide the same solution as the one listed in Table 2 ($v_6 = v_4 = v_2 = 1$, $v_5 = v_3 = v_1 = -1$). Additionally, while $C \times v = 0$ has one degree of freedom by necessity, $\lambda = -1$ has a multiplicity of 1 in $|\lambda \times I - A| = 0$ (indeed, see Example 2).

$C \times v = 0$ from Table 7 has two degrees of freedom (diagonalization produced two zeroes on the main diagonal of matrix C in Table 7, v_5 and v_6 in $C \times v$), so any arbitrary value ($v_5 \cdot v_6 \neq 0$, since it must be $v \neq 0$) of its associated variable will provide an eigenvalue. For instance, $v_5 \leftarrow 1$ and $v_6 \leftarrow 0$ will provide the same solution as the one listed in Table 2 ($v_6 = v_3 = 0$, $v_5 = v_2 = 1$, $v_4 = v_1 = -1$). Furthermore, while $C \times v = 0$ has two degrees of freedom by necessity, $\lambda = 0$ has a multiplicity of 2 in $|\lambda \times I - A| = 0$ (indeed, see Example 2).

Table 6. Diagonalization of $-1 \cdot I - A$ (Table 2, Example 2).

B	1	2	3	4	5	6	C	1	2	3	4	5	6
1	−1	−1	−2	−3	−2	−1	1	1	0	0	0	0	1
2	−1	−1	−1	−2	−3	−2	2	0	1	0	0	0	−1
3	−2	−1	−1	−1	−2	−3	3	0	0	1	0	0	1
4	−3	−2	−1	−1	−1	−2	4	0	0	0	1	0	−1
5	−2	−3	−2	−1	−1	−1	5	0	0	0	0	1	1
6	−1	−2	−3	−2	−1	−1	6	0	0	0	0	0	0

$$C \times \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{bmatrix} = \begin{bmatrix} v_1 + v_6 \\ v_2 - v_6 \\ v_3 + v_6 \\ v_4 - v_6 \\ v_5 + v_6 \\ 0 \end{bmatrix}$$

$B \leftarrow -1 \cdot I - A$; C from Algorithm 3 on B .

Table 7. Diagonalization of $0 \cdot I - A$ (Table 2, Example 2).

B	1	2	3	4	5	6	C	1	2	3	4	5	6
1	0	−1	−2	−3	−2	−1	1	1	0	0	0	1	1
2	−1	0	−1	−2	−3	−2	2	0	1	0	0	−1	0
3	−2	−1	0	−1	−2	−3	3	0	0	1	0	0	−1
4	−3	−2	−1	0	−1	−2	4	0	0	0	1	1	1
5	−2	−3	−2	−1	0	−1	5	0	0	0	0	0	0
6	−1	−2	−3	−2	−1	0	6	0	0	0	0	0	0

$$C \times \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{bmatrix} = \begin{bmatrix} v_1 + v_5 + v_6 \\ v_2 - v_5 \\ v_3 - v_6 \\ v_4 + v_5 + v_6 \\ 0 \\ 0 \end{bmatrix}$$

$B \leftarrow 0 \cdot I - A$; C from Algorithm 3 on B.

Algorithm 4 shows inverse iteration.

Inverse iteration appears to have originally been developed by *Ernst Pohlhausen* [23] with the purpose of computing resonance frequencies in structural mechanics.

If $\kappa_i \in \mathbb{K}$ is not an eigenvalue of A, then $(A - \kappa_i \times I)$ is invertible. The eigenvectors of $(A - \kappa_i \times I)^{-1}$ are the same as the eigenvectors of A, and the corresponding eigenvalues are $\{(\lambda_j - \kappa_i)^{-1}\}$, where $\{\lambda_j\}$ are the eigenvalues of A.

If $\kappa_i \leftarrow \lambda_i - \epsilon$, with λ_i the eigenvalue of A, and ϵ being very small, then $(\lambda_i - \kappa_i)^{-1}$ is much larger than $(\lambda_j - \kappa_i)^{-1}$ for all $j \neq i$. Thus, Algorithm 2 (principal eigenvector) on $(A - \kappa_i I)^{-1}$ will converge rapidly. This idea is called inverse iteration and is implemented as Algorithm 4.

Algorithm 4 Inverse iteration to eigenspaces

Input: A, v //a square diagonalizable matrix A and its eigenvalues v

procedure INVIT(A, w)

$n \leftarrow$ COUNT(A); $E\_Eps \leftarrow 10^{-4}$; $w \leftarrow w - E\_Eps$

$v \leftarrow$ INITV($n, -1$) // $v \leftarrow$ RAND

For($i \leftarrow 0$; $i < n$; $i \leftarrow i + 1$) $A[i][i] \leftarrow A[i][i] - w$ EndFor

GAUSSJ(A, B, C); PRINCIPAL(B, v); RETURN(v) // v is an eigenvector of w

end procedure

$m \leftarrow$ COUNT(v); For($i \leftarrow 0$; $i < m$; $i \leftarrow i + 1$) $u[i] \leftarrow$ INVIT($A, v[i]$) EndFor

Output: u // eigenvectors of A

Taking into consideration the data from Example 2 again, the output of Algorithm 4 is given in Table 8.

One should notice that, for the multiple eigenvalues ($\lambda \in \{-4, 0\}$) of A from Table 2, the solution provided from diagonalization ($v_5 \leftarrow 1$ and $v_6 \leftarrow 0$ in Tables 5 and 7, respectively, eigenvectors in Table 2) and the solution provided by inverse iteration (Table 8) are different, but belong to the same eigenspace ($v_5 \leftarrow -1$ and $v_6 \leftarrow -2$ in Table 5 for the eigenvector associated with the -4 eigenvalue in Table 8; $v_5 \leftarrow 1$ and $v_6 \leftarrow -2$ in Table 7

for the eigenvector associated with the 0 eigenvalue in Table 8). Of course, this is due to the presence of the random effect (see RAND in Algorithm 4).

Table 8. Algorithm 4 output for Example 2 eigenproblem.

Eigenvalue	Eigenvector	Wrong Eigenvector
-4	$[-1 \;\; 1 \;\; 2 \;\; 1 \;\; -1 \;\; -2]^{\mathrm{T}}$	$[1 \;\; 1 \;\; 1 \;\; 1 \;\; 1 \;\; 1]^{\mathrm{T}}$
-1	$[-1 \;\; 1 \;\; -1 \;\; 1 \;\; -1 \;\; 1]^{\mathrm{T}}$	$[1 \;\; 1 \;\; 1 \;\; 1 \;\; 1 \;\; 1]^{\mathrm{T}}$
0	$[1 \;\; 1 \;\; -2 \;\; 1 \;\; 1 \;\; -2]^{\mathrm{T}}$	$[1 \;\; 1 \;\; 1 \;\; 1 \;\; 1 \;\; 1]^{\mathrm{T}}$
9	$[1 \;\; 1 \;\; 1 \;\; 1 \;\; 1 \;\; 1]^{\mathrm{T}}$	$[1 \;\; 1 \;\; 1 \;\; 1 \;\; 1 \;\; 1]^{\mathrm{T}}$
	$v \leftarrow$ RAND in Algorithm 4	$v \leftarrow 1$ in Algorithm 4

The RAND has been used instead of a fixed value initialization, because if (by any chance) the initial eigenvector ($v \leftarrow \text{INITV}(n, -1)$ in Algorithm 4) is colinear with an eigenvector of another eigenvalue (and $[1 \;\; 1 \;\; 1 \;\; 1 \;\; 1 \;\; 1]^{\mathrm{T}}$ is the eigenvector of the 9 eigenvalue, see Table 8), then the convergence fails (see Table 8).

Formally, given a diagonalizable matrix, A, inverse iteration [21] will iterate an approximate eigenvector ($v_{i,k+1}$) when an approximation, κ_i ($\kappa_i \leftarrow \lambda_i - \epsilon$, ϵ small), to a corresponding eigenvalue (λ_i) is used to form $(A - \kappa_i \times I)^{-1}$ (Equation 8), being conceptually similar to the power method (Equation 7). Inverse iteration starts with a random vector, $v_{i,0}$, associated with a λ_i eigenvalue and uses the recurrence relation 8 ($k = 0, 1, \ldots$).

$$v_{i,k+1} \leftarrow \frac{(A - \kappa_i \times I)^{-1} \times v_{i,k}}{\|(A - \kappa_i \times I)^{-1} \times v_{i,k}\|} \tag{8}$$

For big systems, the direct calculation of the characteristic polynomial roots (via Algorithm 1, for instance) may be more than a processor with simple or double precision floating point numbers can handle. Of course, one alternative is to increase the precision, but another alternative is to use a method that adjusts the eigenvalue and the eigenvector at the same time. A modification to the inverse method will provide such an alternative. It should be noted that an approximation of the eigenvalue can be obtained from $\kappa_{i,k+1} \leftarrow v_{i,k}^T \times A \times v_{i,k}$, and then the initialization is $v_{i,0} \leftarrow$ RAND and $\kappa_{i,0} \leftarrow \lambda_i - \epsilon$, and relation (8) is changed into system (9) (Rayleigh quotient iteration, or Ritz method [24]).

$$\begin{cases} v_{i,k+1} \leftarrow \dfrac{(A - \kappa_{i,k} \times I)^{-1} \times v_{i,k}}{\|(A - \kappa_{i,k} \times I)^{-1} \times v_{i,k}\|} \\ \kappa_{i,k+1} \leftarrow v_{i,k+1}^T \times A \times v_{i,k+1} \end{cases} \quad k = 0, 1, \ldots \tag{9}$$

Other aspects of inverse iteration are discussed in [25].

Algorithm 5 shows reducing complexity.

The complexity of the eigenproblem is a function of the dimension of the matrix (n; $n = 6$ in Example 2). If m is the number of (distinct) eigenvalues, then generally $1 \leq m \leq n$ ($m = 4$ in Example 2). The complexity of the eigenproblem is reduced if, instead of finding eigenvalues of A, one finds the eigenvalues of a smaller matrix, of size m. At the same time, m is the smallest size of a matrix that still contains the same eigenvalues. A series of studies [26–30] were dedicated to achieving the goal of reducing the complexity in finding the eigenvalues. The idea is to obtain the biggest orthogonal *Krylov subspace* [31] of A by following a *Gram–Schmidt orthogonalization* [32]. The recipe is given as Algorithm 5.

Algorithm 5 outputs an orthonormal basis (B) of A from which there immediately is an upper Hessenberg matrix ($B^H \times A \times B$) [33], which is, in the case of symmetrical A, a tridiagonal matrix [34].

Consider again Example 2. Table 9 shows that, in the upper Hessenberg matrix (C in Table 9) from the Lanczos–Arnoldi simplification (Algorithm 5), the eigenvalues are preserved from A to $\text{LANCARNO}(A)$. Orthonormal basis (B in Table 9) can be used to derive another matrix ($D \leftarrow B \times B^H$; see Table 9) preserving all eigenvalues and almost

all eigenvectors. Specifically, only eigenvectors corresponding to $\lambda = 0$ are corrupted in Table 9 (see interior eigenvalues in [35–38], exterior eigenvalues in [39–42]). It should be noted that D ($B \times B^H$) contains a non-singular minor of size m (number of distinct eigenvalues of A). However, due to the loss of precision, Krylov-subspace-based methods must often be accompanied by sophisticated subalgorithms implementing restart and orthogonality checking [43]. Variants include the generalized minimal residual algorithm (or Saad–Schultz [30]) and restarted versions [44–47].

Algorithm 5 Lanczos–Arnoldi simplification

Input: A //a square matrix A
procedure LANCARNO(A)
$n \leftarrow$ COUNT(A); $M\_Eps \leftarrow 10^{-7}$; $Q \leftarrow$ INITV($n, -1$) // ${Q^T}_0 \leftarrow$ RAND
For($j \leftarrow 0$; ; $j \leftarrow j+1$)
For($i \leftarrow 0$; $i < n$; $i \leftarrow i+1$) $v[i][0] \leftarrow Q[i][j]$ EndFor // $v \leftarrow {Q^T}_j$
$v \leftarrow$ MULTM(A, v) // $v \leftarrow A \times v$
For($i \leftarrow 0$; $i < n$; $i \leftarrow i+1$) $Q[i][j+1] \leftarrow v[i][0]$ EndFor // ${Q^T}_{j+1} \leftarrow v$
For($i \leftarrow 0$; $i < j$; $i \leftarrow i+1$)
$z \leftarrow 0$; For($k \leftarrow 0$; $k < n$; $k \leftarrow k+1$) $z \leftarrow z + Q[k][i] \cdot Q[k][j+1]$ EndFor
For($k \leftarrow 0$; $k < n$; $k \leftarrow k+1$) $Q[k][j+1] \leftarrow Q[k][j+1] - z \cdot Q[k][i]$ EndFor
EndFor
If (LENV($Q, j+1$) $< M\_Eps$) RETURN(Q) EndIf
EndFor
end procedure
$B \leftarrow$ LANCARNO(A) // B orthonormal basis of A; ${B^H}_{i,j} = \overline{{B^T}_{i,j}}$
Output: B // $B^H \times A \times B$ smallest matrix with same eigenvalues as A

The approximated eigenvectors of A ($B \times v_{\lambda,C}$ in Table 9) are usually obtained from the eigenvectors of the Hessenberg matrix ($v_{\lambda,C}$ in Table 9), multiplied with the orthonormal basis (B in Table 9).

A matrix with distinct eigenvalues has eigenvectors that are linearly independent (as is C in Table 9). As a consequence, the orthonormal basis of that matrix is a square matrix that is also invertible, and an important related property is proven in [48]. The *Cayley transform* [49], which is a mapping between skew-symmetric matrices ($A \in \mathbb{C}$ *skew-Hermitian* $\iff A^H = -A$; $A \in \mathbb{R}$ *skew-symmetric* $\iff A^T = -A$) and orthonormal matrices, is helpful in this instance [50].

Generally, if $A \in \mathbb{R}$ is non-singular and C is from *Cholesky factorization* [51] $A^n \times (A^n)^T \rightarrow C \times C^T$ for $n > 0$, then $C^{-1} \times A$ is orthogonal and convergent to X, for which $X \times A \times X^{-1}$ is triangular. If A is also symmetric, then X is the modal matrix, and a fast algorithm for the calculation of the modal matrix is given in [52].

The Lanczos–Arnoldi simplification (Algorithm 5) can be applied directly (to A), while other approaches employ a preconditioning (of A). Thus, in [53–55], a *Chebyshev polynomial* [56] preconditioner is applied.

Algorithm 6 is combining Algorithms 1, 2, 4, and 5.

If x_0 is an initial approximation of a dominant eigenvector of A, then $A^k x_0$ ($k = 1, 2, \dots$) converges to the dominant eigenvector of A. This is the ***power method*** employed in finding the dominant eigenvectors, and a normalized version of it is given as Equation (7) in Algorithm 2. It is possible to combine the previously given Algorithms 1, 2, 4, and 5, as given in Algorithm 6.

Table 9. Algorithm 5 output for Example 2 eigenproblem.

B	1	2	3	4		
1	0.1343	0.5233	0.2189	−0.3653		
2	0.3728	0.0801	0.5625	0.3963		
3	0.6986	−0.3754	0.1871	−0.4940		
4	0.1868	0.4351	0.2263	0.4448		
5	0.1259	0.6241	−0.2965	−0.3543		
6	0.5516	0.0041	−0.6794	0.3771		
C	1	2	3	4		
1	6.268	4.379	0	0		
2	4.379	1.637	2.017	0		
3	0	2.017	−2.906	0.209		
4	0	0	0.209	−1		
D	1	2	3	4	5	6
1	0.473	0.071	0.119	0.14	0.408	−0.21
2	0.071	0.619	0.14	0.408	−0.21	−0.027
3	0.119	0.14	0.908	−0.21	−0.026	0.071
4	0.14	0.408	−0.21	0.473	0.071	0.119
5	0.408	−0.21	−0.026	0.071	0.618	0.14
6	−0.21	−0.027	0.071	0.119	0.14	0.908
λ	$v_{\lambda,C}$					
9	$[-0.85\ -0.52\ -0.05\ -0.00]^{\mathrm{T}}$					
−4	$[0.14\ -0.32\ 0.92\ -0.18]^{\mathrm{T}}$					
−1	$[0.49\ -0.77\ -0.29\ 0.27]^{\mathrm{T}}$					
0	$[-0.12\ 0.16\ 0.26\ 0.95]^{\mathrm{T}}$					
λ	$v_{\lambda,D}$					
9	$[1\ 1\ 1\ 1\ 1\ 1]^{\mathrm{T}}$					
−4	$[0\ 1\ 1\ 0\ -1\ -1]^{\mathrm{T}}$					
−1	$[1\ -1\ 1\ -1\ 1\ -1]^{\mathrm{T}}$					
0	$[-0.7\ 0.3\ 0.2\ -0.3\ 0.5\ 0.1]^{\mathrm{T}}$					
0	$[0.3\ 0.6\ -0.6\ -0.3\ 0.2\ -0.3]^{\mathrm{T}}$					
0	$[0.2\ 0.1\ 0.2\ -0.7\ -0.4\ 0.6]^{\mathrm{T}}$					
λ	$B \times v_{\lambda,C}$					
9	$[-0.41\ -0.41\ -0.41\ -0.41\ -0.41\ -0.41]^{\mathrm{T}}$					
−4	$[0.00\ 0.50\ 0.50\ 0.00\ -0.50\ -0.50]^{\mathrm{T}}$					
−1	$[-0.41\ 0.41\ -0.41\ 0.41\ -0.41\ 0.41]^{\mathrm{T}}$					
0	$[0.37\ 0.20\ -0.57\ 0.37\ 0.20\ -0.57]^{\mathrm{T}}$					

$B \leftarrow \textsc{LancArno}(A)$, A from Example 2; $B \in \mathbb{R}^{6\times 6}$, so $B^H = B^T$; $C \leftarrow B^H \times A \times B$; $D \leftarrow B \times B^H$; $(\lambda, v_{\lambda,C})$: eigenpair; $(\lambda, v_{\lambda,D})$: eigenpair; $0 \cong A \times B \times v_{\lambda,C} - \lambda \times I$.

Algorithm 6 Rayleigh–Ritz

Input: A //a square matrix A

procedure RR(A)

$B \leftarrow \textsc{LancArno}(A)$; $C \leftarrow B^H \times A \times B$; $P \leftarrow \textsc{Faddeev}(A)$; $R \leftarrow Roots(P)$

$\epsilon \leftarrow 10^{-7}$; $k \leftarrow \textsc{count}(R)$

For($i \leftarrow 0$; $i < k$; $i \leftarrow i + 1$) $\kappa_i \leftarrow R_i - \epsilon$; $D_i \leftarrow (C - \kappa_i \times I)^{-1}$; $\textsc{Principal}(D_i, V_i)$ EndFor

$E \leftarrow B^H \times V$; $\textsc{return}(E)$

end procedure

$E \leftarrow \mathrm{RR}(A)$ // $E_1, E_2, \ldots, E_n$ eigenvectors of A

Output: E // E modal matrix of A

If some authors run variants of Algorithm 5 twice in order to keep away from dangerous eigenvalues [57], in Algorithm 6, the Lanczos–Arnoldi simplification (Algorithm 5)

is iterated once. Even though the resulted matrix (C in Algorithm 6) is not singular, its transformations (D_i) are, and they allow extraction of the eigenvectors one by one. An orthonormal basis (B) allows reverting back to the initial dimensionality ($k \rightarrow n$).

Algorithm 7 shows Jacobi–Davidson.

The Jacobi–Davidson method (given as Algorithm 7), introduced in [58] and based on Jacobi's work [59], rediscovered in [60] and revised in [61], is considered to be one of the best eigenvalue solvers, especially for eigenvalues in the interior of the spectrum [62].

Algorithm 7 Jacobi–Davidson

Input: A //a square matrix A
$x \leftarrow \text{UNITV}(v); y \leftarrow Ax; z \leftarrow x^*y; V[1] \leftarrow [x]; W[1] \leftarrow [y]; H[1] \leftarrow z$
$u \leftarrow x; \theta \leftarrow z; r \leftarrow y - \theta u$
For(;;)
For($k = 1; k < m; k \leftarrow k + 1$)
Solve for x: $(I - uu^*)(A - \theta I)(I - uu^*)x + r = 0$
Orthogonalize x against $V[k]$; $V[k+1] \leftarrow \text{CONCATENATE}(V[k], x))$
$y \leftarrow Ax; W[k+1] \leftarrow \text{CONCATENATE}(V[k], y))$
Compute k^{th} column of $AV[k]$; Compute k^{th} row and column of $H_k \leftarrow V[k]^*AV[k]$
Compute the largest eigenpair (θ, s) of $H[k+1]$; $s \leftarrow \text{UNITV}(s)$
$x \leftarrow V[k+1]s; y \leftarrow Ax; r \leftarrow y - \theta u$ //Ritz vector
If($\text{ABS}(r) < \epsilon$) RETURN //stop if convergence
$V[1] \leftarrow [u]; W[1] \leftarrow [y]; H[1] \leftarrow [\theta]$ //restart
EndFor
EndFor
Output: (θ, u) // θ approximates τ

Algorithm 8 shows Gauss–Seidel.

The Gauss–Seidel method (given as Algorithm 8) is an iterative method used to solve a system of linear equations, appearing for the first time in [63].

Algorithm 8 can be applied to any matrix with nonzero elements on the diagonals, but convergence is only guaranteed if the matrix is either strictly diagonally dominant, or symmetric and positive definite [64].

Algorithm 8 Gauss–Seidel

Input: A, u, v //Solve iteratively $Au = v$
$n \leftarrow \text{COUNT}(u)$
For ($k = 1; ; k \leftarrow k + 1$)
$w \leftarrow u$
For (i = 1; $i < n; i \leftarrow i + 1$)
$u[i] \leftarrow v[i]$
For (j = 1; $j < n; j \leftarrow j + 1$) If($i <> j$) $u[i] \leftarrow u[i] - A[i][j]u[j]$; EndIf EndFor
$u[i] \leftarrow u[i]/A[i][i]$
EndFor
If($\text{ABS}(u - w) < \epsilon$) BREAK
EndFor
Output: u // Solution of $Au = v$

4. The QR, QL, RQ, and LQ (or Francis–Kublanovskaya) Decompositions

The QR algorithm or QR iteration is an eigenvalue algorithm: that is, a procedure to calculate the eigenvalues and eigenvectors of a matrix. The QR algorithm was developed (independently) by Francis [65,66] and Kublanovskaya [67,68]. Even though some people call it Francis' algorithm [69], its proper name should be *Francis–Kublanovskaya*.

The basic idea is to perform a decomposition (of QR, QL, RQ, or LQ type), express the matrix as a product of an orthogonal matrix and an upper triangular matrix, multiply the

factors in the reverse order, and iterate. There are several methods for actually computing the QR decomposition, such as by means of the Gram–Schmidt process, Householder transformations, or Givens rotations. Each has a number of advantages and disadvantages.

The primary literature for QR, QL, RQ, and LQ decompositions in relation to parallelization is [70], while the first algorithm was given in [71].

5. Properties of Eigenvalues

Eigenvalues and eigenvectors are special quantities when related to their precursor entities. One can imagine that the usual space is replaced by another space—eigenspace (Figure 1).

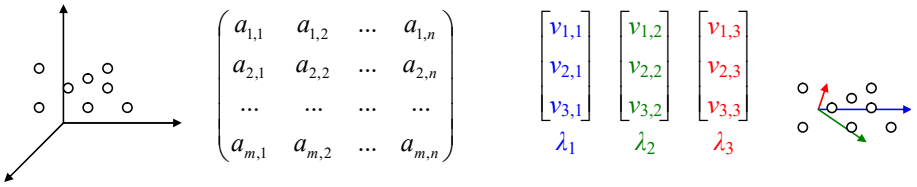
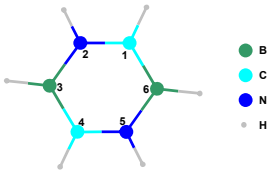


Figure 1. Euclidean space and data (**left**) vs. Eigenspace and features (**right**).

The properties of eigenvalues on orthogonal matrices were studied in [72], on skew-symmetric matrices in [73], and on anti-symmetric matrices in [74]. An explicit solution to the eigenvalue problem of a self-adjoint differential operator with a given set of self-adjoint boundary conditions (in terms of the Green's function, eigenfunctions, and eigenvalues of another problem having the same operator but different boundary conditions) is provided as an extension of the Sturm–Liouville theory in [75].

The method of transplantation was proposed in [76] to be applied if the functional in question is characterized as the extremum value of another functional over a certain function class with respect to the domain of definition. The method was later applied in the theory of torsional rigidity, virtual mass, and conformai radius [76], in the case of the membrane equation and a general problem of electrostatic capacity of a body with a boundary surface and an exterior [77]. Poisson's equation on complete noncompact manifolds with nonnegative Ricci curvature is tackled in [78], and eigenvalues for integral operators in [79]. Random Hermitian matrices, of interest in statistical physics, also reveal peculiar eigenvalue sets in connection with the distribution of prime numbers [80–82].

Undirected and unweighted graphs are just a case often used in molecular sciences [15], and an adjacency matrix, square and symmetric, is the scholastic example (Figure 2), possessing a series of important properties [83].



$|\lambda \cdot [Id] - [Ad]| = 0 \rightarrow |\lambda \cdot [I] - [C]| = 0$

[C]	1	2	3	4	5	6	[I]	1	2	3	4	5	6
1	0	a	e	h	d	c	1	j	0	0	0	0	0
2	a	0	b	d	g	f	2	0	k	0	0	0	0
3	e	b	0	c	f	i	3	0	0	1	0	0	0
4	h	d	c	0	a	e	4	0	0	0	j	0	0
5	d	g	f	a	0	b	5	0	0	0	0	k	0
6	c	f	i	e	b	0	6	0	0	0	0	0	1

Figure 2. From graphs to molecules by generalizing the adjacency and identity matrices.

One important consequence of operating on integer-based matrices is the possibility of extracting the exact values of the characteristic polynomial coefficients one by one (Algorithm 1, Ref. [84]). This, when coupled with a polynomial root finder algorithm [85], becomes a powerful tool for eigenvalue finding [86]. The difference between extreme eigenvalues of a graph is commonly referred to as the spread of the graph [87].

6. Classical Case Studies

Eigenproblems appear in:

- Quantum localization: quantum theory states that the energy levels correspond to the eigenvalues of a Scrödinger operator [88]; when the operator is too complex, it is often replaced by a random Hermitian matrix and its eigenvalues should correspond to the energy levels of the system; the Gaussian orthogonal ensemble and Gaussian unitary ensemble are typical examples of specific instances [89]; quantum mechanics for particle localization [90], quantification of energy [91], magnetic momentum [92], and electronic spin [93], and the complementary problem of geometrical alignment with complex eigenvalues [74];
- Molecular topology [94] utilizes so-called molecular graphs, which use graph theory to operate on molecular structures. Characterizing molecular graphs is a matter of whether a graph has a certain property. The adjacency matrix $A(A_{i,j})$ with entries of 1 if i and j are connected by an edge, otherwise 0. The distance matrix is an extension of it. Another extension is by considering counts of the number of edges for multiple edges and negative integers for directed graphs. In all instances, a characteristic polynomial can be built [15];
- Vibrations of bars and strings [95], and more general to wave propagation [96];
- Laplace's equation (and its generalizations, Poisson and Helmholtz's equations), or the potential theory of harmonic functions, in problems involving electrostatic fields, heat conduction, shapes of films and membranes, gravitation and hydrodynamics [97];
- The Sturm–Liouville problem [98], with particular cases to Bessel and Legendre's equations and the complementary problem of nuclear collisions with complex eigenvalues [99];
- Stability analysis of systems characterized by sets of ordinary differential equations [100];
- Electrical circuits emulating eigenproblems [101].

7. Applications

Matrices of quaternions [102] require special treatment regarding the eigenvalues. Actually, there are two eigenproblems to be solved, left ($Ax = \lambda x$, [103]) and right ($Ax = x\lambda$, [104]). The right eigenproblem has its solutions invariant under the similar transformation [105].

Spectral decomposition uses eigenvalues [106] and is involved in the analysis of variance. For the covariance matrix of the errors, see [107]. For the variability of a tensor-valued random variable, see [108]. For Lamb waves decomposition, see [109]. For nonparametric forecasting of data, see [110]. The fact that the state of a bilinear control system can be split uniquely into generalized modes corresponding to the eigenvalues of the dynamics matrix is proven in [106].

In electric circuits, high impedance faults can be identified by inspecting the eigenvalue space of the circuit [111]. Thus, stability analysis can rely on the calculation of the eigenvalues [112]. The stability of different systems is inspected this way: wind turbines in [113], fluids with non-parallel flow in [114], impedance- and admittance-based electrical systems in [115], three-wheel vehicles in [116], and polynomially dependent one-parameter systems in general in [117].

Classical multivariate analysis considers vectors $v \in \mathbb{R}^m$, such that for all $u \in \mathbb{R}^m$, $u^T v$ is a univariate normal, while v establishes the m-variate normal distribution with $\mu \leftarrow E(v)$ as mean and $\Sigma = E((v-\mu)(v-\mu)^T)$ as covariance. The Wishart matrix $W \leftarrow A^T A$, computed from an n by m matrix, A, collecting n samples, defines the Wishart distribution. An important property of the Wishart distribution is that it is the sampling distribution of the maximum likelihood estimator (MLE) of the covariance matrix of a multivariate normal distribution [118]. Eigenvalues of a matrix are informative about matrix structure, thus the eigenvalues of the sample covariance matrices give information about the underlying distribution [119].

Principal component analysis (PCA, [120]) is a way of identifying patterns in data, and expressing the data in such a way so as to highlight their similarities and differences. In doing so, it reduces the dimensionality of a data set based on calculating eigenvectors and eigenvalues of the input data (Algorithm 9).

Algorithm 9 First Principal Component

Input: A //a data matrix with zero mean, A
procedure FPC(A, c, B)
$x \leftarrow$ RAND; $x \leftarrow$ UNITV(x) // Random initialization
For ($j = 0; j <$ COLS(A); $j \leftarrow j + 1$) //For each column of data
$y \leftarrow 0$; For ($i = 0; i <$ ROWS(A); $i \leftarrow i + 1$)$y \leftarrow y + (A[i]x)A[i]$ EndFor
$c \leftarrow x^T y$; $x \leftarrow$ UNITV(y); If(ABS($cx - y$) $< \epsilon$) EXIT
EndFor
end procedure
CPC(A, c, B) // B is the first principal component
Output: c, B // eigenvalue and its eigenvector

Once the first component is extracted, the algorithm (Algorithm 9) can easily be adapted to extract the rest of the components.

Dominant component analysis is a PCA variation meant to extract an orthogonal set of data descriptors in relation to an dependent variable [121]. Discriminant component analysis is a PCA variation provided as a feature extraction scheme for face recognition [122]. Factor analysis is another variation from PCA designed to identify certain unobservable factors from the observed variables [123]. In PCA, one rewrites the samples on the basis of the eigenvectors. The components of the vector so formed are the principal components and their variances are eigenvalues [124]. In data of high dimensions, where the luxury of graphical representation is not available, PCA is a powerful tool for analyzing data. Another use of PCA is for data compressing: once patterns in data are identified, reducing the number of dimensions without much loss of information is possible.

Image compression [125], denoising [126], and recognition [127] perform eigenvector decomposition, which is very useful in computer tomography [128], magnetic resonance [129], and polarized light [130] imaging, stratigraphic mapping [131], lidar [132], and radar [133].

Principal component regression ([134], PCR) is a regression based on PCA in which the principal components of the explanatory variables are used as regressors. In some instances, large sets of independent variables are available (7 in [135], 13 in [136], 4536 in [88], 576,288 in [15], a maximum number of 787,968 in [137–139], or even 2,387,280 in [140,141]. One of the strategies of deriving models for the dependent variable(s) is to perform a full (preferred in [15,137]), heuristic (preferred in [138,139]), random (preferred in [140]), or combined (preferred in [141]) search, while other approaches extract principal components from the pool of independent variables (preferred in [135,136]) and, in other instances, grouping and classification based on the principal components is desired (as in [88]).

Quantum localization is, in the end, a problem of optimization. A less-known fact is that the BFGS (from Broyden, Fletcher, Goldfarb, and Shanno, see [142–145]) algorithm, as well as other built-in algorithms for quantum localization, such as the DFP (from Davidon, Fletcher, and Powell, see [146–148]) and the steepest descent method [149], are closely related to the calculation of the eigenvalues [150]. Several recent modifications [151–154] make them even more versatile in unconstrained nonlinear optimization.

8. Conclusions and Perspectives

Eigenproblem basics and algorithms are revised from a historical perspective. Many problems may be formulated as eigenproblems, and both classical cases as well as many other discovered applications contain a large pool of variate uses. Several classical eigenvalue and eigenvector calculation algorithms are given and their use is exemplified.

More and more eigenproblem algorithms are stated every day. In [155], the authors propose selection procedures that improve spectral clustering algorithms in high-dimensional settings. The use of a trimmed sampling algorithm applied on the eigenvalues is proposed in [156] to replace the iterated eigenvalues for localization problems of large quantum systems. In [157], an iterative algorithm is proposed for the extraction of analytic eigen-

vectors for decomposition of parahermitian matrices arising in broadband multiple-input multiple-output systems or array processing.

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Appendix A. Algorithms Involved in Eigenproblem Basic Operations

Below can be found some algorithms for basic operations on vectors and matrices, which were referred to in the algorithm given in the main part of the work.

Algorithm A1 Constructing unity (square) matrix

Input: n //dimension of the expected square matrix
  function UNITM(n)
    For($i \leftarrow 0; i < n; i \leftarrow i+1$) For($j \leftarrow 0; j < n; j \leftarrow j+1$) $A[i][j] = 0$ EndFor EndFor
    For($i \leftarrow 0; i < n; i \leftarrow i+1$) $A[i][i] = 1$ EndFor
    RETURN(A) // $A \leftarrow I_n$
  end function
  $I \leftarrow$ UNITM(n) // $I \leftarrow I_n$
Output: I // I is the unity matrix over $\mathbb{K}^{n \times n}$

Algorithm A2 Adding two matrices

Input: A, B //matrices
  function ADDM($\&A, \&B$)
    $n \leftarrow$ COUNT(A); $m \leftarrow$ COUNT($A[0]$)
    For($i \leftarrow 0; i < n; i \leftarrow i+1$) For($j \leftarrow 0; j < m; j \leftarrow j+1$)
      $C[i][j] = A[i][j] + B[i][j]$
    EndFor EndFor
    RETURN(C) // $C \leftarrow A + B$
  end function
  $C \leftarrow$ ADDM(A, B) // $C \leftarrow A + B$
Output: C // $C \leftarrow A + B$

Algorithm A3 Multiplication with a scalar

Input: c, A //c scalar, A matrix
  function MULTC($\&c, \&A$)
    $n \leftarrow$ COUNT(A); $m \leftarrow$ COUNT($A[0]$)
    For($i \leftarrow 0; i < n; i \leftarrow i+1$) For($j \leftarrow 0; j < m; j \leftarrow j+1$)
      $B[i][j] = c \cdot A[i][j]$
    EndFor EndFor
    RETURN(B) // $B \leftarrow c \cdot A$
  end function
  $B \leftarrow$ MULTC(c, A) // $B \leftarrow c \cdot A$
Output: B // $B \leftarrow c \cdot A$

Algorithm A4 Multiplication of two matrices

Input: A, B //A, B square matrices

function MULTM(&A, &B)

$n1 \leftarrow$ COUNT(A); $n2 \leftarrow$ COUNT$(A[0])$; $n3 \leftarrow$ COUNT(B); $n4 \leftarrow$ COUNT$(B[0])$

If($n2 \neq n3$) DIE("Multiplication not possible.") EndIf

For($i \leftarrow 0$; $i < n1$; $i \leftarrow i + 1$) For($j \leftarrow 0$; $i < n4$; $j \leftarrow j + 1$)

$C[i][j] \leftarrow 0$

For($k \leftarrow 0$; $i < n2$; $k \leftarrow k + 1$) $C[i][j] \leftarrow C[i][j] + A[i][k] \cdot B[k][j]$ EndFor

EndFor EndFor

RETURN(C) // $C \leftarrow A \times B$

end function

$C \leftarrow$ MULTM(A, B) // $C \leftarrow A \times B$

Output: C // $C \leftarrow A \times B$

Algorithm A5 Trace of a (square) matrix

Input: A //A square matrix

function TRACE(&A)

$n \leftarrow$ COUNT(A); $r \leftarrow 0$; For($i \leftarrow 0$; $i < n$; $i \leftarrow i + 1$) $r \leftarrow r + A[i][i]$ EndFor

RETURN(r) // $r \leftarrow Tr(A)$

end function

$c \leftarrow$ TRACE(A) // $c \leftarrow Tr(A)$

Output: c // $B \leftarrow Tr(A)$

Algorithm A6 Init a vector

Input: n, t //n - size of the vector; t - type/value of initialization

function INITV(n, t)

If($t \geq 0$)

For($i \leftarrow 0$; $i < n$; $i \leftarrow i + 1$) $v[i][0] \leftarrow t$ EndFor // $v \leftarrow t$

Else

For($i \leftarrow 0$; $i < n$; $i \leftarrow i + 1$) $v[i][0] \leftarrow$ RAND EndFor // $v \leftarrow$ RAND

EndIf

end function

$v \leftarrow$ INITV(n, t) // v is an initialized vector

Output: v // v is an initialized vector

Algorithm A7 Length of a vector stored in a column

Input: v, k //$v_{\cdot,k}$ line vector

function LENV(&v)

$n \leftarrow$ COUNT(v); $r \leftarrow 0$

For($i \leftarrow 0$; $i < n$; $i \leftarrow i + 1$) $r \leftarrow r + v[i][k] \cdot v[i][k]$ EndFor

$r \leftarrow \sqrt{r}$; RETURN(r) // $r \leftarrow \|v_{\cdot,k}\|_{\text{Euclidean}}$

end function

$w \leftarrow$ LENV(v) // $w \leftarrow \|v_{\cdot,k}\|_{\text{Euclidean}}$

Output: w // $w \leftarrow \|v_{\cdot,k}\|_{\text{Euclidean}}$

Algorithm A8 Direction of a vector

Input: v //v line vector

function UNITV(&v)

$n \leftarrow$ COUNT(v); $w \leftarrow$ LENV$(v, 0)$; $u \leftarrow$ MULTC$(1/w, v)$

RETURN(u) // $u \leftarrow v/\|v\|_{\text{Euclidean}}$

end function

$u \leftarrow$ UNITV(v) // $u \leftarrow v/\|v\|$

Output: u // $u \leftarrow v/\|v\|$

Algorithm A9 Absolute difference of two vectors

Input: v, w //v,w line vectors

function ADIFFV(&v, &w)

$n \leftarrow$ COUNT(v); $r \leftarrow 0$

For($i \leftarrow 0$; $i < n$; $i \leftarrow i + 1$) $r \leftarrow r + |v[i][0] - w[i][0]|$ EndFor

RETURN(r) // $r \leftarrow \|v - w\|_{\text{Manhattan}}$

end function

$d \leftarrow$ ADIFFV(v, w) // $d \leftarrow \|v - w\|_{\text{Manhattan}}$

Output: d // $d \leftarrow \|v - w\|_{\text{Manhattan}}$

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