Eigensystems

We will discuss matrix diagonalization algorithms in *Numerical Recipes* in the context of the eigenvalue problem in quantum mechanics,

\[ A|n\rangle = \lambda_n |n\rangle, \tag{1} \]

where \( A \) is a real, symmetric Hamiltonian operator and \( |n\rangle \) is the \( n \)-th eigenvector with eigenvalue \( \lambda_n \).

In an \( N \)-dimensional vector space, Eq. (1) becomes

\[ \sum_{j=1}^{N} A_{ij} x_j^{(n)} = \lambda_n x_i^{(n)}, \tag{2} \]

where \( A \) is an \( N \times N \) matrix, and \( x_i^{(n)} \) is the \( i \)-th element of the \( n \)-th eigenvector \( x^{(n)} \in \mathbb{R}^N \).

**ORTHONORMAL BASIS**

(Orthogonality) The basis set \( \{ |n\rangle \}_{n=1,\ldots,N} \) can be made orthonormal, i.e.,

\[ \langle m|n \rangle = \sum_{j=1}^{N} x_j^{(m)} x_j^{(n)} = \delta_{mn}, \tag{3} \]

or, by defining the transformation matrix \( U \) as

\[ U_{in} = x_i^{(n)} \tag{4} \]

(i.e., the \( n \)-th column of \( U \) is the \( n \)-th eigenvector), \( U \) is orthogonal,

\[ U^TU = I \tag{5} \]

where \( I \) is the \( N \times N \) identity matrix.

Proof of Eq. (3): First note that all eigenvalues \( \lambda_n \) are real. (\( \because \) By multiplying eq. (1) by \( \langle n| \) from the left, \( \langle n|A|n \rangle = \lambda_n \langle n|n \rangle \). For a Hermitian matrix (and of course for a real, symmetric matrix), \( \langle n|A|n \rangle \) is real, and \( \langle n|n \rangle \) is also real since its complex conjugate is itself.) Next, by multiplying Eq. (1) by \( \langle m| \) from the left, we obtain

\[ \langle m|A|n \rangle = \lambda_n \langle m|n \rangle. \tag{6} \]

Similarly,

\[ \langle n|A|m \rangle = \lambda_m \langle n|m \rangle. \tag{7} \]

By taking the complex conjugate of Eq. (7) and noting the reality of the eigenvalue,

\[ \langle m|A|n \rangle = \lambda_m \langle m|n \rangle. \tag{8} \]

Subtracting Eq. (8) from Eq. (6),

\[ 0 = (\lambda_n - \lambda_m) \langle m|n \rangle. \tag{9} \]

If \( \lambda_n \neq \lambda_m \), Eq. (9) requires that \( \langle m|n \rangle = 0 \). On the other hand, if \( \lambda_n = \lambda_m \), we can still make them orthogonal without modifying the eigenvalue. For example, Gram-Schmidt orthogonalization procedure
\[ |n'\rangle \leftarrow |n\rangle - |m\rangle \langle m|n\rangle \quad (10) \]

makes \( \langle m|n'\rangle = \langle m|n\rangle - \langle m|m\rangle \langle m|n\rangle = \langle m|n\rangle - \langle m|n\rangle = 0 \), followed by the normalization \( |n'\rangle \) as \( |n'\rangle \leftarrow |n'\rangle/\langle n'|n'\rangle^{1/2} \).

(Completeness) The orthonormal basis set \( \{|n\rangle\} \) is also complete, i.e., in the \( N \)-dimensional vector space,

\[ \sum_{n=1}^{N} |n\rangle \langle n| = 1 \quad (11) \]

is the identity operator. Equivalently,

\[ \sum_{n=1}^{N} x_{i}^{(n)} x_{j}^{(n)} = \delta_{ij} \quad (12) \]

or

\[ UU^{T} = I \quad (13) \]

Equation (11) states that any vector in the \( N \)-dimensional vector space \( |\psi\rangle \) is a linear combination of the \( N \) basis functions,

\[ |\psi\rangle = \sum_{n=1}^{N} |n\rangle \langle n|\psi\rangle \quad (14) \]

since there are only \( N \) linearly independent vectors in this vector space.

The orthogonality and completeness together states that

\[ U^{T}U = UU^{T} = I \quad (15) \]

or

\[ U^{-1} = U^{T} \quad (16) \]

**ORTHOGONAL TRANSFORMATION**

Now, we use the orthogonal matrix \( U \) to restate the matrix eigenvalue problem. To do so, multiply Eq. (2) by \( x_{i}^{(m)} \) and sum the resulting equation over \( i \),

\[ \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} x_{j}^{(n)} = \lambda_{n} \sum_{i=1}^{N} x_{i}^{(m)} x_{i}^{(n)} = \lambda_{n} \delta_{mn} \quad (17) \]

where we have used the orthonormality, Eq. (3). Using \( U \), equation (17) can be rewritten as

\[ U^{T} A U = \Lambda \quad (18) \]

where

\[ \Lambda_{mn} = \lambda_{n} \delta_{mn} \quad (19) \]

is a diagonal matrix. Thus the matrix eigenvalue problem amounts to finding an orthogonal matrix, \( U \), or the associated orthogonal transformation, Eq. (18), which eliminates all the off-diagonal matrix elements.
GRAND STRATEGY

The grand strategy of matrix diagonalization is to nudge the matrix $A$ towards diagonal form by a sequence of orthogonal transformations,

$$ A \rightarrow P_1^T A P_1 \rightarrow P_2^T P_1^T A P_1 P_2 \rightarrow \ldots, $$

so that its off-diagonal elements gradually disappear. At the end, the orthogonal matrix is

$$ U = P_1 P_2 \cdots. $$

ORTHOGONAL TRANSFORMATION ~ ROTATION: JACOBI TRANSFORMATION

As an illustration, let us consider a two-state system, for which the most general Hamiltonian matrix is

$$ H = \begin{bmatrix} \varepsilon_1 & \delta \\ \delta & \varepsilon_2 \end{bmatrix}. $$

(We define the indices such that $\varepsilon_1 < \varepsilon_2$, i.e., the first state is the lower-energy state.) We express first eigenvector of this Hamiltonian as

$$ |u\rangle = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} = \cos \theta |1\rangle + \sin \theta |2\rangle, $$

which is most general. (Because of the normalization condition, the any vector in the 2-dimensional vector space can be specified by one parameter.) Once we specify the first eigenvector, the second is readily determined from the orthonormality as

$$ |v\rangle = \begin{bmatrix} -\sin \theta \\ \cos \theta \end{bmatrix}, $$

see the figure below. The rotation angle $\theta$ specifies the deviation of the first eigenvector $|u\rangle$ from $|1\rangle$.

The orthogonal matrix is then

$$ U = \begin{bmatrix} u & v \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}. $$

To find the specific rotation angle $\theta$, let us return to the original eigenvalue problem,

$$ \begin{bmatrix} \lambda - \varepsilon_1 & -\delta \\ -\delta & \lambda - \varepsilon_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. $$

The eigenvalues are obtained by solving the secular equation,
\[
\det(\lambda I - H) = \begin{vmatrix} \lambda - \epsilon_1 & -\delta \\ -\delta & \lambda - \epsilon_2 \end{vmatrix} = (\lambda - \epsilon_1)(\lambda - \epsilon_2) - \delta^2 = 0,
\]
and its two solutions are
\[
\lambda_{\pm} = \frac{\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4\delta^2}}{2}.
\]
Now let us examine the lower eigenenergy \(\lambda_{\pm}\). By substituting the eigenvalue and the corresponding eigenvector, Eq. (22), into Eq. (24), we obtain
\[
\theta = \tan^{-1}\left(\frac{-\epsilon_1 + \epsilon_2 - \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4\delta^2}}{2\delta}\right).
\]
For example, if the off-diagonal element \(\delta\) is small, we can expand Eq. (27) into its power series, the first term of which is (we have assumed \(\epsilon_1 < \epsilon_2\))
\[
\theta = \frac{\delta}{\epsilon_1 - \epsilon_2}.
\]

**Jacobi Transformation**

In Jacobi transformation, each orthogonal transformation \(P_i\) in Eq. (20) is the two-dimensional rotation applied to a pair of rows, \(i\) and \(j\), and the pair of columns of the same indices. One such rotation eliminates a pair — \((i, j)\) and \((j, i)\) — of off-diagonal elements. A sequence of two-dimensional rotations will eventually eliminate all the off-diagonal elements. (In fact, later rotations may partially restore off-diagonal elements eliminated earlier. Nevertheless, this procedure will converge, and the square sum of all the off-diagonal elements becomes smaller as we continue the procedure.)

**HOUSEHOLDER TRANSFORMATIONS FOR TRIDIAGONALIZATION**

Instead of eliminating a pair of off-diagonal elements at one time as in Jacobi transformation, Householder transformation eliminates an entire row but the first two elements at a time.

In Chapter 11 of *Numerical Recipes*, Householder transformations are used to reduce a real, symmetric matrix to a tridiagonal form, in which only the diagonal \((A_{ii})\), upper subdiagonal \((A_{i+1,i})\), and lower subdiagonal \((A_{i,i+1})\) elements may be nonzero. The function \texttt{tred2()} achieves this. The resulting tridiagonal matrix is then diagonalized (i.e., both subdiagonal elements are eliminated), using another sets of orthogonal transformations in function \texttt{tqli()}. The magical orthogonal matrix \(P\) is constructed from a vector in the \(N\)-dimensional vector space. First, let us prove a useful lemma.

(Lemma) Let \(v \in \mathbb{R}^N\) and
\[
P = I - \frac{2vv^T}{v^Tv},
\]
then \(P\) is symmetric and orthogonal, i.e.,
\[
P^TP = PP = I.
\]
First,\[ P_{ij} = \delta_{ij} - 2v_i v_j \sum_{k=1}^{2} v_k^2, \] is symmetric with respect to the exchange of the indices \( i \) and \( j \). Next,\[
P^T P = \left( I - \frac{2vv^T}{v^Tv} \right) \left( I - \frac{2vv^T}{v^Tv} \right)
= I - \frac{4vv^T}{v^Tv} + \frac{4vv^T vv^T}{(v^Tv)^2} \quad \text{//}
= I - \frac{4vv^T}{v^Tv} + \frac{4vv^T}{v^Tv} = I
\]

Now, given an arbitrary vector \( x \) in the \( N \)-dimensional vector space, we can device an orthogonal matrix that eliminates all the elements but the first one when multiplied to \( x \).

(Theorem) For \( \forall x \in \mathbb{R}^N \), let\[
v = x \pm \| x \|_2 e_1
\] where\[
e_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}
\] and the vector 2-norm is defined as\[
\| x \|_2 = \sqrt{x^T x} = \sqrt{\sum_{i=1}^{N} x_i^2}.
\] Then\[
P x = \left( I - \frac{2vv^T}{v^Tv} \right) x = \mp \| x \|_2 e_1,
\] i.e., the Householder matrix \( P \), when multiplied, eliminates all the elements of \( x \) but the first one.

Note that,\[
v^Tv = \left( x^T \pm \| x \|_2 e_1^T \right) \left( x \pm \| x \|_2 e_1 \right)
= \| x \|_2^2 \pm 2\| x \|_2 x_1 + \| x \|_2^2
= 2\| x \|_2^2 (\| x \|_2 \pm x_1)
\] Then
\[ PX = x - \frac{2vv^T}{2\|x\|_2^2 (\|x\|_2 \pm x_1)}x \]
\[ = x - \frac{(x \pm \|x\|_2 e_1)(x^T \pm \|x\|_2 e_1^T)x}{\|x\|_2^2 (\|x\|_2 \pm x_1)} \] 

//
\[ = x - \frac{(x \pm \|x\|_2 e_1)(\|x\|_2 \pm x_1)}{\|x\|_2 (\|x\|_2 \pm x_1)} \]
\[ = x - x \mp \|x\|_2 e_1 = \mp \|x\|_2 e_1 \]

The Householder matrix can be used for tridiagonalization as follows: Let us decompose a real, symmetric matrix \( A \) as
\[
A = \begin{bmatrix}
  a_{11} & a_{12} & \cdots & a_{1N} \\
  a_{21} & \ddots & & \vdots \\
  \vdots & & \ddots & \vdots \\
  a_{N1} & & & a_{NN}
\end{bmatrix} = \begin{bmatrix}
  a_{11} & A_{12} = A_{21}^T \\
  A_{21} & A_{22}
\end{bmatrix}.
\] (36)

where \( A_{21}, A_{12}, \) and \( A_{22} \) are \((N-1)\times1, 1\times(N-1), \) and \((N-1)\times(N-1)\) matrices, respectively. Now let
\[
v = (\in \mathbb{R}^{N-1}) = A_{21} + \text{sign}(a_{21})\|A_{21}\|_2 e_1.
\] (37)

(The sign has been chosen to minimize the cancellation error.) Then
\[
\overline{P}A_{21} = \left( I_{N-1} - \frac{2vv^T}{v^Tv} \right)A_{21} = -\text{sign}(a_{21})\|A_{21}\|_2 e_1 = k e_1.
\] (38)

Now
\[
PAP = \begin{bmatrix}
  1 & 0 & \cdots & 0 \\
  \vdots & \ddots & & \vdots \\
  0 & & \ddots & \vdots \\
  0 & & & 1
\end{bmatrix}
\begin{bmatrix}
  a_{11} & A_{21}^T \\
  A_{21} & A_{22}
\end{bmatrix}
\begin{bmatrix}
  1 & 0 & \cdots & 0 \\
  \vdots & \ddots & & \vdots \\
  0 & & \ddots & \vdots \\
  0 & & & 1
\end{bmatrix}
\]
\[= \begin{bmatrix}
  a_{11} & \overline{P}A_{21} \\
  k & \overline{P}A_{22}
\end{bmatrix}
\begin{bmatrix}
  1 & 0 & \cdots & 0 \\
  \vdots & \ddots & & \vdots \\
  0 & & \ddots & \vdots \\
  0 & & & 1
\end{bmatrix},
\] (39)

i.e., all the elements in the first row and first column but \( a_{11}, a_{12}, \) and \( a_{21} \) have been eliminated by this transformation. Next, a similar Householder transformation is applied to the first column and first row of the \((N-1)\times(N-1)\) submatrix \( \overline{P}A_{22} \overline{P} \), which eliminates all the elements in the second row and second column in the original \( N \times N \) matrix but \( a_{22}, a_{23}, \) and \( a_{32}, \) so on (see the figure below, in which white cells represent eliminated matrix elements).
After \((N-2)\) such transformations, all the off-diagonal elements but the diagonal and upper/lower sub-diagonal elements are eliminated.

**DIAGONALIZATION OF A TRIDIAGONAL MATRIX—QR DECOMPOSITION**

**QR Decomposition**

The diagonalization of the tridiagonal matrix obtained above can use QR decomposition (or similar QL decomposition). That is, any square matrix \(A\) can be decomposed into

\[
A = QR,
\]

where \(Q\) is an orthogonal matrix and \(R\) is an upper-triangular matrix, i.e., \(R_{ij} = 0\) for \(i > j\).

For example, this can be achieved by using a Householder transformation as follows. First, we decompose the \(N\times N\) matrix \(A\) into the first column \(A_1\) and the rest \(A_2\):

\[
A = \begin{bmatrix}
a_{11} \\
\vdots \\
a_{N1}
\end{bmatrix} = \begin{bmatrix}
A_1 \\
A_2
\end{bmatrix}.
\]  

(41)

Let

\[
v \in \mathbb{R}^N = A_1 + \text{sign}(a_{11})\|A_1\|_2 e_1,
\]

then

\[
PA_1 = \left( I_N - \frac{2vv^T}{v^Tv} \right) A_1 = -\text{sign}(a_{11})\|A_1\|_2 e_1 = ke_1,
\]

(43)

and thus

\[
PA = \begin{bmatrix}
PA_1 & PA_2 \\
0 & \vdots & PA_2 \\
0 & \vdots & \vdots & \ddots & \vdots \\
0 & \vdots \\
0
\end{bmatrix}
\]

(44)

i.e., all the elements in the first column but one have been eliminated. Next, we can apply a similar elimination to \(A(2:N,2:N)\) submatrix to eliminate all the lower-triangular elements in the second column, see the figure below.

After \((N-1)\) transformation, the resulting matrix is upper-triangular, i.e.,
\[ P_{N-1} \cdots P_2 P_1 A = R, \quad (45) \]

or

\[ P_1^{-1} P_2^{-1} \cdots P_{N-1}^{-1} R = QR. \quad (46) \]

**Orthogonal Transformation**

Let Eq. (40) be the QR decomposition of matrix \( A \). Then, define another matrix by

\[ A' = RQ. \quad (48) \]

Since \( R = Q^{-1}A = Q^T A \) from Eq. (40), Eq. (48) defines an orthogonal transformation,

\[ A \rightarrow A' = Q^T AQ. \quad (49) \]

It can be proven that, if \( A \) is tridiagonal, then \( A' \) is also tridiagonal, i.e., the orthogonal transformation preserves the tridiagonality. The QR algorithm consists of successive applications of this orthogonal transformation.

(QR algorithm)

\[
\begin{align*}
1. & \quad Q_s R_s \leftarrow A_s \\
2. & \quad A_{s+1} \leftarrow R_s Q_s, \quad s = 1, 2, \ldots .
\end{align*}
\quad (50)
\]

The following theorems then guarantee that the eigenvalues and eigenvectors can be obtained by the QR algorithm.

(Theorem)

1. \( \lim_{s \to \infty} A_s \) is upper-triangular, and
2. The eigenvalues appear on its diagonal.

In Chapter 11 of *Numerical Recipes*, function \( \text{tqli()} \) uses QL algorithm, instead of the above QR algorithm, to achieve lower-triangularity, to minimize the cancellation error.