

Eigensystems

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

$$A|n\rangle = \lambda_n|n\rangle, \quad (1)$$

where A is a real, symmetric Hamiltonian operator and $|n\rangle$ is the n -th eigenvector with eigenvalue λ_n . In an N -dimensional vector space, Eq. (1) becomes

$$\sum_{j=1}^N A_{ij}x_j^{(n)} = \lambda_n x_i^{(n)}, \quad (2)$$

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

ORTHONORMAL BASIS

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

$$\langle m|n\rangle \equiv \sum_{i=1}^N x_i^{(m)} x_i^{(n)} = \delta_{mn}, \quad (3)$$

or, by defining the transformation matrix U as

$$U_{in} = x_i^{(n)} \quad (4)$$

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

$$U^T U = I \quad (5)$$

where I is the $N \times N$ identity matrix.

Proof of Eq. (3): First note that all eigenvalues λ_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

$$\langle m|A|n\rangle = \lambda_n \langle m|n\rangle. \quad (6)$$

Similarly,

$$\langle n|A|m\rangle = \lambda_m \langle n|m\rangle. \quad (7)$$

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

$$\langle m|A|n\rangle = \lambda_m \langle m|n\rangle. \quad (8)$$

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

$$0 = (\lambda_n - \lambda_m) \langle m|n\rangle. \quad (9)$$

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

$$U^T U = U U^T = I. \quad (15)$$

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 ,

$$\sum_{i=1}^N \sum_{j=1}^N x_i^{(m)} A_{ij} x_j^{(n)} = \lambda_n \sum_{i=1}^N x_i^{(m)} x_i^{(n)} = \lambda_n \delta_{mn}, \quad (17)$$

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

$$U^T A U = \Lambda, \quad (18)$$

where

$$\Lambda_{mn} = \lambda_m \delta_{mn}, \quad (19)$$

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,

$$A \rightarrow P_1^T A P_1 \rightarrow P_2^T P_1^T A P_1 P_2 \rightarrow \dots, \quad (20)$$

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

$$U = P_1 P_2 \dots. \quad (21)$$

ORTHOGONAL TRANSFORMATION ~ ROTATION: JACOBI TRANSFORMATION

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

$$H = \begin{bmatrix} \varepsilon_1 & \delta \\ \delta & \varepsilon_2 \end{bmatrix}. \quad (22)$$

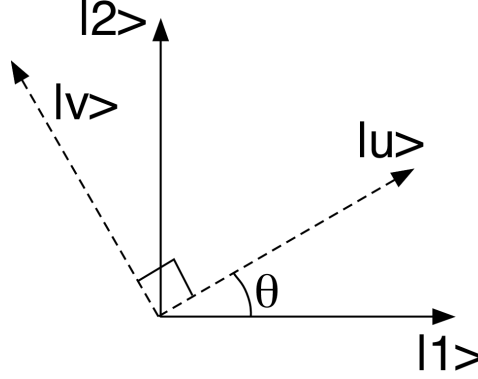
(We define the indices such that $\varepsilon_1 < \varepsilon_2$, i.e., the first state is the lower-energy state.) We express first eigenvector of this Hamiltonian as

$$|u\rangle = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} = \cos\theta |1\rangle + \sin\theta |2\rangle, \quad (22)$$

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

$$|v\rangle = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}, \quad (22)$$

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



The orthogonal matrix is then

$$U = [u \quad v] = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}. \quad (23)$$

To find the specific rotation angle θ , let us return to the original eigenvalue problem,

$$\begin{bmatrix} \lambda - \varepsilon_1 & -\delta \\ -\delta & \lambda - \varepsilon_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \quad (24)$$

The eigenvalues are obtained by solving the secular equation,

$$\det(\lambda I - H) = \begin{vmatrix} \lambda - \varepsilon_1 & -\delta \\ -\delta & \lambda - \varepsilon_2 \end{vmatrix} = (\lambda - \varepsilon_1)(\lambda - \varepsilon_2) - \delta^2 = 0, \quad (25)$$

and its two solutions are

$$\lambda_{\pm} = \frac{\varepsilon_1 + \varepsilon_2 \pm \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\delta^2}}{2}. \quad (26)$$

Now let us examine the lower eigenenergy λ_- . By substituting the eigenvalue and the corresponding eigenvector, Eq. (22), into Eq. (24), we obtain

$$\theta = \tan^{-1} \left(\frac{-\varepsilon_1 + \varepsilon_2 - \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\delta^2}}{2\delta} \right). \quad (27)$$

For example, if the off-diagonal element δ is small, we can expand Eq. (27) in its power series, the first term of which is (we have assumed $\varepsilon_1 < \varepsilon_2$)

$$\theta = \frac{\delta}{\varepsilon_1 - \varepsilon_2}. \quad (28)$$

Jacobi Transformation

In Jacobi transformation, each orthogonal transformation P_k 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 ($A_{i,i+1}$), and lower subdiagonal ($A_{i+1,i}$) elements may be nonzero. The function `tridiagonalize()` achieves this. The resulting tridiagonal matrix is then diagonalized (i.e., both subdiagonal elements are eliminated), using another set of orthogonal transformations in function `tridiagonalize()`.

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

$$P = I - \frac{2vv^T}{v^Tv}, \quad (29)$$

then P is symmetric and orthogonal, i.e.,

$$P^T P = P P = I. \quad (30)$$

∴First,

$$P_{ij} = \delta_{ij} - \frac{2v_i v_j}{\sum_{k=1}^N v_k^2}, \quad (31)$$

is symmetric with respect to the exchange of the indices i and j . Next,

$$\begin{aligned} P^T P &= \left(I - \frac{2vv^T}{v^Tv} \right) \left(I - \frac{2vv^T}{v^Tv} \right) \\ &= I - \frac{4vv^T}{v^Tv} + \frac{4vv^T vv^T}{(v^Tv)^2} \quad // \\ &= I - \frac{4vv^T}{v^Tv} + \frac{4vv^T}{v^Tv} = I \end{aligned}$$

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

$$v = x \pm \|x\|_2 e_1 \quad (32)$$

where

$$e_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (33)$$

and the vector 2-norm is defined as

$$\|x\|_2 = \sqrt{x^T x} = \sqrt{\sum_{i=1}^N x_i^2}. \quad (34)$$

Then

$$Px = \left(I - \frac{2vv^T}{v^Tv} \right) x = \mp \|x\|_2 e_1, \quad (35)$$

i.e., the Householder matrix P , when multiplied, eliminates all the elements of x but the first one.

∴Note that,

$$\begin{aligned}
v^T v &= (x^T \pm \|x\|_2 e_1^T)(x \pm \|x\|_2 e_1) \\
&= \|x\|_2^2 \pm 2\|x\|_2 x_1 + \|x\|_2^2 \\
&= 2\|x\|_2(\|x\|_2 \pm x_1)
\end{aligned}$$

Then

$$\begin{aligned}
Px &= x - \frac{2vv^T}{2\|x\|_2(\|x\|_2 \pm x_1)} x \\
&= x - \frac{(x \pm \|x\|_2 e_1)(x^T \pm \|x\|_2 e_1^T)x}{\|x\|_2(\|x\|_2 \pm x_1)} \quad // \\
&= x - \frac{(x \pm \|x\|_2 e_1)\|x\|_2(\|x\|_2 \pm x_1)}{\|x\|_2(\|x\|_2 \pm x_1)} \\
&= x - x \mp \|x\|_2 e_1 = \mp \|x\|_2 e_1
\end{aligned}$$

The Householder matrix can be used for tridiagonalization as follows: Let us decompose a real, symmetric matrix A as

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & & & \\ \vdots & & & \\ a_{N1} & & & \end{bmatrix} = \begin{bmatrix} a_{11} & A_{12} = A_{21}^T & \\ A_{21} & A_{22} & \end{bmatrix}. \quad (36)$$

where A_{21} , A_{12} , and A_{22} are $(N-1) \times 1$, $1 \times (N-1)$, and $(N-1) \times (N-1)$ matrices, respectively. Now let

$$v \in \mathbf{R}^{N-1} = A_{21} + \text{sign}(a_{21})\|A_{21}\|_2 e_1. \quad (37)$$

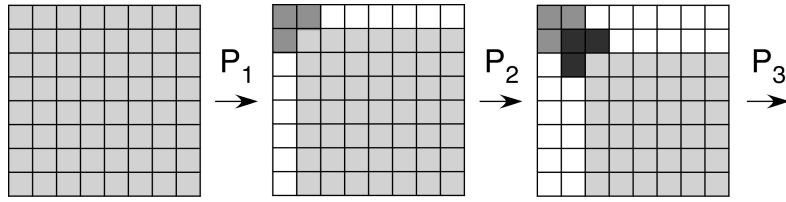
(The sign has been chosen to minimize the cancellation error.) Then

$$\bar{P}A_{21} \equiv \left(I_{N-1} - \frac{2vv^T}{v^T v}\right)A_{21} = -\text{sign}(a_{21})\|A_{21}\|_2 e_1 \equiv ke_1. \quad (38)$$

Now

$$\begin{aligned}
PAP &\equiv \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & & \\ 0 & & & \end{bmatrix} \begin{bmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & & \\ 0 & & & \end{bmatrix} \\
&\quad \begin{bmatrix} a_{11} & A_{21}^T \\ k & \bar{P}A_{22} \\ 0 & \\ \vdots & \\ 0 & \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & & \\ 0 & & & \end{bmatrix}, \quad (39) \\
&\quad \begin{bmatrix} a_{11} & k & 0 & \cdots & 0 \\ k & & & & \\ 0 & & \bar{P}A_{22}\bar{P} & & \\ \vdots & & & & \\ 0 & & & & \end{bmatrix}
\end{aligned}$$

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 $\bar{P}A_{22}\bar{P}$, 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

$$A = QR, \quad (40)$$

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 :

$$A = \begin{bmatrix} a_{11} \\ \vdots \\ a_{N1} \end{bmatrix} = \begin{bmatrix} A_1 & A_2 \end{bmatrix}. \quad (41)$$

Let

$$v \in R^N = A_1 + \text{sign}(a_{11})\|A_1\|_2 e_1, \quad (42)$$

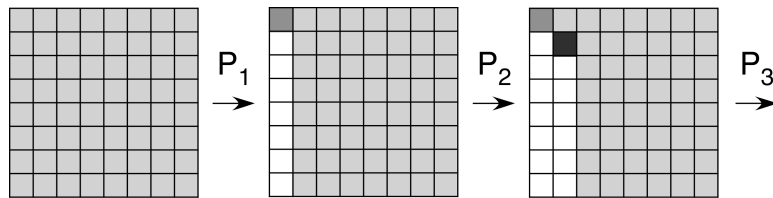
then

$$PA_1 \equiv \left(I_N - \frac{2vv^T}{v^T v}\right) A_1 = -\text{sign}(a_{11})\|A_1\|_2 e_1 \equiv ke_1, \quad (43)$$

and thus

$$PA = \begin{bmatrix} PA_1 & PA_2 \end{bmatrix} = \begin{bmatrix} k & \\ 0 & PA_2 \\ \vdots & \\ 0 & \end{bmatrix}, \quad (44)$$

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

$$A = P_1^{-1} P_2^{-1} \cdots P_{N-1}^{-1} R \equiv QR. \quad (46)$$

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,

$$A \rightarrow A' = Q^T A Q. \quad (49)$$

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)

$$\begin{cases} 1. & Q_s R_s \leftarrow A_s \\ 2. & A_{s+1} \leftarrow R_s Q_s \end{cases} \quad s = 1, 2, \dots \quad (50)$$

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

(Theorem)

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

In Chapter 11 of *Numerical Recipes*, function `tqli()` uses QL algorithm, instead of the above QR algorithm, to achieve lower-triangularity, to minimize the cancellation error. It diagonalizes a tridiagonal matrix by applying a sequence of rotations to eliminate the subdiagonal elements.