Jacobi Algorithm for Real Symmetric Matrices:-

1. At each step, find the largest off-diagonal element, say S_{pq} (Alternately, cycle through each off-diagonal index (p,q), one at a time).

2. find an orthogonal matrix J such that with

$$S' = J^T S J$$

S' has $(S')_{pq} = 0$.

↳ We will see how to do this in a moment.

3. Check if the "relative error" is less than the desired error.

If not, repeat steps 1 & 2.

i.e., stop if $\frac{\mathrm{off}(S)}{|S|} < \varepsilon$ where ε is the desired accuracy bound.

else, continue.

How find the matrix J?

find a 2×2 matrix. $R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$

such that

$$R(\theta)^T \begin{pmatrix} S_{pp} & S_{pq} \\ S_{qp} & S_{qq} \end{pmatrix} R(\theta) \quad \text{is}$$

a 2×2 diagonal matrix,

say $\begin{pmatrix} S'_{pp} & 0 \\ 0 & S'_{qq} \end{pmatrix}$.

Then let J be the matrix,

$J_{kk} = 1$ unless $k = p$ or $k = q$.

$J_{pp} = \cos\theta = J_{qq}$

$J_{pq} = \sin\theta$

$J_{qp} = -\sin\theta$

$J_{ij} = 0$ for $i \neq j$ and if $(i,j) \neq (p,q)$ or (q,p).

In other words,

$$J = \begin{pmatrix} 1 & & & & & & 0 \\ & \ddots & & & & & \\ & & \cos\theta & \cdots & \sin\theta & & \\ & & \vdots & \ddots & \vdots & & \\ & & -\sin\theta & \cdots & \cos\theta & & \\ & & & & & \ddots & \\ 0 & & & & & & 1 \end{pmatrix}.$$

Now suppose after K steps, we reach the desired accuracy, i.e

$$\text{off}(S') < \epsilon |S'| \quad \text{where}$$

$$S' = J_K^T \cdots J_2^T J_1^T S J_1 J_2 \cdots J_K.$$

where $J_1, J_2 \ldots J_K$ are the orthogonal matrices generated in steps $1, 2 \ldots K$.

Then the desired orthogonal matrix is $O = J_1 J_2 \cdots J_K$ and it's columns are the desired eigenvectors.

Next, we will turn to complex Hermitian matrices.

Complex Matrix Diagonalization :-

A complex vector

$$\begin{pmatrix} z_1 \\ \vdots \\ z_N \end{pmatrix} = \begin{pmatrix} x_1 + i y_1 \\ \vdots \\ x_N + i y_N \end{pmatrix}$$ can be

represented as a $2N \times 1$ real vector

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \\ y_1 \\ \vdots \\ y_N \end{pmatrix}.$$

Now a 1×1 matrix (i.e a scalar).

$\alpha = a + ib$ transforms z to.

$$z' = (ax - by) + i(ay + bx).$$

Thus if $z' = x' + iy'$, then

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.$$

(Here, a, b, x, y, x', y' are all reals).

Thus a complex matrix $C = A + iB$ where A and B are real. can be represented as

$$\begin{pmatrix} A & -B \\ B & A \end{pmatrix}$$

If $H = H_r + i H_{im}$ where H_r and H_{im} are real matrices. and H is Hermitian, i.e., $(H^T)^* = H$,

then one can easily verify that

$$H' = \begin{pmatrix} H_r & -H_{im} \\ H_{im} & H_r \end{pmatrix}$$ is a real symmetric matrix.

Thus, one can use the method for diagonalizing real symmetric matrices for the complex Hermitian case.

Note, in the complex case, one should use orthogonal matrices which are also of the form $\begin{pmatrix} A & -B \\ B & A \end{pmatrix}$

One can check that if

$$O = \begin{pmatrix} O_r & -O_{im} \\ O_{im} & O_r \end{pmatrix}$$ is orthogonal,

i.e $O\, O^T = \mathbb{1} \Rightarrow O_r O_r^T + O_{im} O_{im}^T = \mathbb{1}$

and $O_r O_{im}^T - O_{im} O_r^T = 0$

then $U = O_r + i O_{im}$ is unitary, i.e

$$U U^{\dagger} = \mathbb{1}$$

This is guaranteed by choosing J of the form discussed earlier for making $(H')_{pq} = 0$

In the end, H' should have the form

$$\begin{pmatrix} \lambda_1 & & & & & & & \\ & \lambda_2 & & & & & & \\ & & \ddots & & & & & \\ & & & \lambda_N & & & & \\ & & & & \lambda_1 & & & \\ & & & & & \lambda_2 & & \\ & & & & & & \ddots & \\ & & & & & & & \lambda_N \end{pmatrix}.$$

which correspond to the

eigenvalues $\lambda_1 \ldots \ldots \lambda_N$

The first N columns of the

orthogonal matrix $O = J_1 J_2 \ldots J_K$ give

the eigen-vectors.

If $\begin{pmatrix} u \\ \hdashline v \end{pmatrix} \begin{matrix} \}N \\ \}N \end{matrix}$ is the p^{th} column, then

the complex vector $(u + iv)\}N$ is an

eigenvector of H'.