For a symmetric matrix A, an eigenvector v is a vector that satisfies

$$A.v = \lambda v$$

the corresponding eigenvalue

For an $N \times N$ matrix there are N eigenvectors $v_1, v_2, v_3, \dots v_N$ with corresponding eigenvalues $\lambda_1, \lambda_2, \lambda_3, \dots \lambda_N$

The eigenvectors are orthogonal

$$v_i . v_j = 0 \quad \text{if } i \neq j$$

and they are normalized

$$v_i . v_i = 1$$ (this is just convention)

If we consider the matrix V, where each column is an eigenvector v, we can write all N equations

$$A v_i = \lambda_i v_i$$

into a single equation

$$\boxed{A.V = V.D}$$

where D is a diagonal matrix with the eigenvalues λ_i.

Because the eigenvectors are orthogonal, the matrix V is orthogonal

$$V^T V = V V^T = \mathbb{1}$$

QR ALGORITHM is a popular techique to diagonalize real symmetric and Hermitian matrices

(diagonalize = find eigenvalues and eigenvectors)

The algorithm uses the QR decomposition of the matrix. We will details about the decomposition next. For now we just need to know that this is a way to break the matrix A into the product

$$\underbrace{Q}_{\text{orthogonal matrix}} \cdot \underbrace{R}_{\text{upper-triangular matrix}}$$

⇒ Let us start by writing

$$\boxed{A = Q_1 . R_1}$$

⇒ multiply by Q_1^T

$$Q_1^T A = \underbrace{Q_1^T \, Q_1}_{\mathbb{1}} R_1 = R_1$$

⇒ Define a new matrix

$$A_1 = \underbrace{R_1}_{} . Q_1$$

from above $R_1 = Q_1^T A$

$$\boxed{A_1 = Q_1^T A \, Q_1}$$

⇒ Repeat the process

$$\boxed{A_1 = Q_2 . R_2}$$

$$\underbrace{Q_2^T A_1}_{} = R_2$$

new matrix

$$A_2 = R_2 . Q_2$$

$$\boxed{A_2 = Q_2^T A_1 Q_2}$$

so

$$A_2 = Q_2^T \, Q_1^T \, A \, Q_1 \, Q_2$$

⇛ Repeating the process many times

$$A_1 = Q_1^T \, A \, Q_1$$

$$A_2 = Q_2^T \, Q_1^T \, A \, Q_1 \, Q_2$$

$$A_3 = Q_3^T \, Q_2^T \, Q_1^T \, A \, Q_1 \, Q_2 \, Q_3$$

$$\cdots$$

$$A_k = \left(Q_k^T \ldots Q_1^T \right) A \left(Q_1 \ldots Q_k \right)$$

⇛ It can be proven that if we continue this process long enough, the matrix A_k will eventually become diagonal. The off-diagonal elements become smaller and smaller the more iterations we do.

In practice, A_k is approximately a diagonal matrix D

⇛ Let us define

$$V = Q_1 . Q_2 . Q_3 \ldots Q_k$$

From above

$$V^T A \, V = D$$

multiplying by V

$$\boxed{AV = VD}$$

which is exactly the original equation we had to solve.

Therefore

•) The diagonal elements of

$$A_k = \left(Q_k^T \dots Q_1^T\right) A \left(Q_1 \dots Q_k\right)$$

are the eigenvalues

•) Each column of

$$V = Q_1 . Q_2 . Q_3 \dots Q_k$$

is an eigenvector

RECIPE

1) Create an $N \times N$ identity matrix V.
Choose the target accuracy ϵ for the off-diagonal elements of the eigenvalue matrix

2) Calculate the QR decomposition

$$A = QR \quad \text{(see below how to do it)}$$

3) Update A to the new value

$$A = R.Q$$

4) Multiply V on the right by Q

$$V = V.Q$$

5) Check the off-diagonal elements of the new A. If they are less than ϵ, we are done. Otherwise go back to step 2.

QR decomposition

⇒ Let us think of A as a set of N column vectors $a_0, a_1, \ldots a_{N-1}$

using Python numbering

⇒ Let us define two sets of vectors

$u_0, u_1, \dots u_{N-1}$ and $q_0, q_1 \cdots q_{N-1}$

$$\begin{cases} u_0 = a_0 \\ u_1 = a_1 - (q_0 \cdot a_1)\, q_0 \\ u_2 = a_2 - (q_0 \cdot a_2)\, q_0 - (q_1 \cdot a_2)\, q_1 \\ \dots \end{cases}$$

$$q_0 = \frac{u_0}{|u_0|} \qquad q_1 = \frac{u_1}{|u_1|} \qquad q_2 = \frac{u_2}{|u_2|}$$

General formulas

$$\boxed{u_i = a_i - \sum_{j=0}^{i-1} (q_j \cdot a_i)\, q_j}$$

$$\boxed{q_i = \frac{u_i}{|u_i|}}$$

⇒ It can be shown that the vectors q_i are

ORTHONORMAL

$\{ 1 \quad$ if $i \neq j$

$$q_i \cdot q_j = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

$\Rightarrow$) Rearranging the definitions

$$\begin{cases} a_0 = |u_0|\, q_0 \\ a_1 = |u_1|\, q_1 + (q_0 . a_1)\, q_0 \\ a_2 = |u_2|\, q_2 + (q_0 . a_2)\, q_0 + (q_1 . a_2)\, q_1 \\ \ldots \end{cases}$$

$\Rightarrow$) This can be written in a matrix form

$$A = \begin{pmatrix} | & | & | \\ a_0 & a_1 & a_2 \\ | & | & | \end{pmatrix} = \underbrace{\begin{pmatrix} | & | & | \\ q_0 & q_1 & q_2 \\ | & | & | \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} |u_0| & q_0 . a_1 & q_0 . a_2 \\ 0 & |u_1| & q_1 . a_2 \\ 0 & 0 & |u_2| \end{pmatrix}}_{R}$$

orthogonal matrix

upper triangular matrix

This is the Q R decomposition.

(1) Starting with a certain matrix A, we use the v's and q's

above to write $\quad A_{old} = QR$

(2) Update

$$A_{new} = RQ$$

.) If the process is repeated, use A_{new} above and its corresponding new v's and q's to get new Q and R and restart the steps (1) and (2)