Similarity Transformations and diagonalization

Monday, October 21, 2024 11:26

Change of basis

Consider a vector $\vec{x}$ in an N-dimensional space & let $\{\hat{e}_i\}_{i=1}^{N}$ be an orthonormal basis set

$$\vec{x} = x_1\hat{e}_1 + x_2\hat{e}_2 + \dots + x_N\hat{e}_N$$

Think of $\{\hat{e}_i\}_{i=1}^{N}$ as the primitive orthonormal basis

$$\hat{e}_1 = \begin{pmatrix}1\\0\\0\\\vdots\\0\end{pmatrix}, \quad \hat{e}_2 = \begin{pmatrix}0\\1\\0\\\vdots\\0\end{pmatrix}, \quad \hat{e}_N = \begin{pmatrix}0\\0\\0\\\vdots\\1\end{pmatrix}$$

Choose a new basis such that

$$\hat{e}_j' = \sum_{i=1}^{N} S_{ij}\hat{e}_i \qquad \{\text{a new orthonormal basis}\}$$

The components of $\vec{x}$ will also change in the new basis

$$\vec{x} = \sum_{i=1}^{N} x_i\hat{e}_i = \sum_{j=1}^{N} x_j'\hat{e}_j'$$

$$= \sum_{j=1}^{N} x_j' \sum_{i=1}^{N} S_{ij}\hat{e}_i$$

$$= \sum_{i=1}^{N} \underbrace{\sum_{j=1}^{N} S_{ij}x_j'}\,\hat{e}_i$$

$$x_i = \sum_{j=1}^{N} S_{ij}x_j'$$

In matrix form

$$|x\rangle = \hat{S}\,|x'\rangle$$

components of $\vec{x}$ in $\{\hat{e}_i\}$ basis

components of $\vec{x}$ in $\{\hat{e}_i'\}$ basis

Notice, the matrix $\hat{S}$ is just

$$\begin{pmatrix} \vdots & \vdots & \vdots & & \vdots \\ \hat{e}_1' & \hat{e}_2' & \hat{e}_3' & \cdots & \hat{e}_N' \\ \vdots & \vdots & \vdots & & \vdots \end{pmatrix}$$

the elements of $\hat{S}$ are the components of $\hat{e}_j'$ expressed in the primitive basis $\hat{e}_i$

But $\{\hat{e}_j'\}_{j=1}^{N}$ forms a linearly independent basis.

Thus, $\hat{S}^{-1}$ exists.

It follows that: $|x\rangle = \hat{S}\,|x'\rangle$

$$\hat{S}^{-1}\left[\,|x\rangle = \hat{S}\,|x'\rangle\,\right]$$

or $|x'\rangle = \hat{S}^{-1}\,|x\rangle$

Compare this with

$$\hat{e}_j' = \sum_{i=1}^{N} S_{ij}\hat{e}_i \longrightarrow \underbrace{|\hat{e}'\rangle = \hat{S}\,|\hat{e}\rangle}$$

The components & the basis of the same vector $\vec{x}$ transform inversely

Linear system (eigenvector approach)

$$\hat{\mathcal{L}}\,|x\rangle = |y\rangle$$

where $\hat{\mathcal{L}}$ is a linear operator

(which can be represented as a matrix)

$|x\rangle$ unknown vector (or function)

$|y\rangle$ known vector (or function)

Goal: find $|x\rangle$

If $\hat{\mathcal{L}}$ is a normal matrix, then we can use its eigenvectors to span the vector space where $|x\rangle$ and $|y\rangle$ lives.

Let $\{|\hat{e}_n\rangle\}_{n=1}^{N}$ be an orthonormal eigenvectors of $\hat{\mathcal{L}}$

$$\hat{\mathcal{L}}\,|\hat{e}_n\rangle = \lambda_n|\hat{e}_n\rangle$$

Since $\{|\hat{e}_n\rangle\}_{n=1}^{N}$ can span the N-dimensional vector space, then

$$|y\rangle = \sum_{n=1}^{N} y_n|\hat{e}_n\rangle \quad \text{where } y_n \text{ are known coefficients}$$

and

$$|x\rangle = \sum_{n=1}^{N} x_n|\hat{e}_n\rangle \quad \text{where } x_n \text{ are unknown coefficients}$$

It follows that

$$\hat{\mathcal{L}}\,|x\rangle = |y\rangle$$

$$\hat{\mathcal{L}}\left(\sum_{n=1}^{N} x_n|\hat{e}_n\rangle\right) = \sum_{n=1}^{N} y_n|\hat{e}_n\rangle$$

$$\sum_{n=1}^{N} x_n\,\hat{\mathcal{L}}\,|\hat{e}_n\rangle = \sum_{n=1}^{N} y_n|\hat{e}_n\rangle$$

$$\sum_{n=1}^{N} x_n\lambda_n|\hat{e}_n\rangle = \sum_{n=1}^{N} y_n|\hat{e}_n\rangle$$

By using the linear independence of $\{|\hat{e}_n\rangle\}_{n=1}^{N}$ or its orthogonality property,

$$x_n = \frac{y_n}{\lambda_n}$$

Now, consider the linear system

$$\hat{\mathcal{L}}\,|x\rangle = |y\rangle \qquad \hat{\mathcal{L}}'\,|x'\rangle = |y'\rangle$$

component matrix in the old basis

component matrix in the new basis

How does the elements (entries) of $\hat{\mathcal{L}}$ change when the basis is changed?

$$\hat{\mathcal{L}}'\hat{S}^{-1}|x\rangle = \hat{S}^{-1}|y\rangle$$

$$\hat{S}\left[\hat{\mathcal{L}}'\hat{S}^{-1}|x\rangle = \hat{S}^{-1}|y\rangle\right]$$

$$\underbrace{\left[\hat{S}\hat{\mathcal{L}}'\hat{S}^{-1}\right]}|x\rangle = |y\rangle$$

This is just the original linear system with

$$\hat{\mathcal{L}} = \hat{S}\hat{\mathcal{L}}'\hat{S}^{-1} \quad \text{or}$$

$$\left[\hat{\mathcal{L}} = \hat{S}\hat{\mathcal{L}}'\hat{S}^{-1}\right]\hat{S}$$

$$\hat{S}^{-1}\left[\hat{\mathcal{L}}\hat{S} = \hat{S}\hat{\mathcal{L}}'\right]$$

$$\hat{\mathcal{L}}' = \hat{S}^{-1}\hat{\mathcal{L}}\hat{S}$$

(similarity transformation)

$$\hat{S}: \{|\hat{e}_i\rangle\}_{i=1}^{N} \longrightarrow \{|\hat{e}_j'\rangle\}_{j=1}^{N}$$

If we are transforming into two orthonormal basis set,

$\langle\hat{e}_m|\hat{e}_n\rangle = \delta_{mn}$ ✓ $\quad \langle\hat{e}_m'|\hat{e}_n'\rangle = \delta_{mn}$ ✓

NOT necessarily have the ff relations $\langle\hat{e}_m'|\hat{e}_n\rangle = \delta_{mn}$

How to build $\hat{S}$

$$|\hat{e}_j'\rangle = \sum_{i=1}^{N} S_{ij}|\hat{e}_i\rangle$$

$$\langle\hat{e}_m|\left[\,|\hat{e}_j'\rangle = \sum_{i=1}^{N} S_{ij}|\hat{e}_i\rangle\right]$$

$$\langle\hat{e}_m|\hat{e}_j'\rangle = \sum_{i=1}^{N} S_{ij}\langle\hat{e}_m|\hat{e}_i\rangle$$

$$= \sum_{i=1}^{N} S_{ij}\delta_{mi}$$

$$= S_{mj}$$

Thus the elements of $\hat{S}$ is obtained via

$$S_{ij} = \langle\hat{e}_i|\hat{e}_j'\rangle$$

Exercise: Find the similarity transformation from the ff primitive basis:

$$|\hat{e}_1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}, \quad |\hat{e}_2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}, \quad |\hat{e}_3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

to the new orthonormal basis

$$|\hat{e}_1'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}, \quad |\hat{e}_2'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}, \quad |\hat{e}_3'\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$$

Build $\hat{S}$:

$S_{11} = \langle\hat{e}_1|\hat{e}_1'\rangle = \frac{1}{\sqrt{2}}$ $\quad S_{12} = \langle\hat{e}_1|\hat{e}_2'\rangle = \frac{1}{\sqrt{2}}$ $\quad S_{13} = \langle\hat{e}_1|\hat{e}_3'\rangle = 0$

$S_{21} = 0$ $\quad S_{22} = 0$ $\quad S_{23} = 1$

$S_{31} = \frac{1}{\sqrt{2}}$ $\quad S_{32} = -\frac{1}{\sqrt{2}}$ $\quad S_{33} = 0$

Thus,

$$\hat{S} = \begin{array}{c} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \\ \begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ |\hat{e}_1'\rangle & |\hat{e}_2'\rangle & |\hat{e}_3'\rangle \end{array} \end{array}$$

Q1 Consider $\hat{S}$ that will change the orthonormal basis

$$|\hat{e}_1'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-i\end{pmatrix} \quad |\hat{e}_2'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-i\\0\\1\end{pmatrix} \quad |\hat{e}_3'\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$$

to

$$|\hat{e}_1''\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}, \quad |\hat{e}_2''\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad |\hat{e}_3''\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\end{pmatrix}$$

Now that we have constructed $\hat{S}$, we can transform any matrix $\hat{M}$ originally defined in the "old" basis, to its form in the new basis

$$\hat{M}' = \hat{S}^{-1}\hat{M}\hat{S}$$

Q2. Let $\hat{M}' = \begin{pmatrix}0&1&0\\1&0&1\\0&1&2\end{pmatrix}$ as defined in the orthonormal basis set $\{e_n'\}_{n=1}^{3}$. What is the new form of $\hat{M}' \to \hat{M}''$ in the new basis $\{\hat{e}_n''\}_{n=1}^{3}$?