Similarity Transformation and Diagonalization (cont.)

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Properties of similarity transformation

1) The identity matrix is not changed by the similarity transformation

Let $\hat{\mathcal{L}} = \hat{\mathbb{1}}$, then

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

2) The value of the determinant is unchanged.

$$\hat{\mathcal{L}}' = \hat{S}^{-1}\hat{\mathcal{L}}\hat{S}$$
$$\det\left[\hat{\mathcal{L}}' = \hat{S}^{-1}\hat{\mathcal{L}}\hat{S}\right]$$
$$\det(\hat{\mathcal{L}}') = \det(\hat{S}^{-1}\hat{\mathcal{L}}\hat{S})$$
$$= \det(\hat{S}^{-1})\cdot\det(\hat{\mathcal{L}})\cdot\det(\hat{S})$$
$$= \frac{1}{\det(\hat{S})}\cdot\det(\hat{\mathcal{L}})\cdot\det(\hat{S})$$
$$\det(\hat{\mathcal{L}}') = \det(\hat{\mathcal{L}})$$

3) The equation to solve for the eigenvalues of a matrix under similarity transformation is unchanged.

Suppose we are solving for the eigenvalues of $\hat{A}$, then

$$\det(\hat{A} - \lambda\mathbb{1}) = 0$$
$$\det\left[\hat{S}^{-1}(\hat{A} - \lambda\mathbb{1})\hat{S}\right] = 0$$
$$\det(\hat{S}^{-1}\hat{A}\hat{S} - \lambda\hat{S}^{-1}\hat{S}) = 0$$
$$\det(\hat{A}' - \lambda\hat{\mathbb{1}}) = 0$$

4) The trace is unchanged.

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

Recall: similarity transformation maps the old basis to the new basis via

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

* The components of $\vec{x}$ transform as

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

and the elements of a matrix $\hat{\mathcal{L}}$ transform according to

$$\hat{\mathcal{L}}' = \hat{S}^{-1}\hat{\mathcal{L}}\hat{S} \quad \text{(similarity transformation)}$$

Unitary similarity transformation

Some similarity transformations are unitary.

$$\hat{S}^{-1} = \hat{S}^{+} \quad \text{(definition of unitary transformation)}$$

1) The inner-product in the old basis is preserved.

Let $|x\rangle, |y\rangle$ be the components of two vectors in the old basis. In the new basis, we have

$$|x'\rangle = S^{-1}|x\rangle \quad \text{and} \quad |y'\rangle = S^{-1}|y\rangle$$

since $\hat{S}$ is unitary, then

$$|x'\rangle = \hat{S}^{+}|x\rangle \quad \leftarrow \text{unitary}$$
$$\left[|x'\rangle = \hat{S}^{+}|x\rangle\right]^{+}$$
$$\langle x'| = \langle x|\hat{S}.$$

The inner-product of $|x'\rangle$ and $|y'\rangle$ gives

$$\langle x'|y'\rangle = (\langle x|\hat{S})(\hat{S}^{-1}|y\rangle)$$
$$= \langle x|\hat{S}\hat{S}^{-1}|y\rangle$$
$$= \langle x|y\rangle$$

2) Hermitian matrices in the "old" basis remain Hermitian in the "new" basis.

Let $\hat{H}$ be Hermitian in the "old" basis.

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

since $\hat{S}$ is unitary, then $\hat{H}' = \hat{S}^{+}\hat{H}\hat{S}$.

Now, let us take the transpose conjugate

$$\left[\hat{H}' = \hat{S}^{+}\hat{H}\hat{S}\right]^{+}$$
$$\hat{H}'^{+} = \hat{S}^{+}\hat{H}^{+}(\hat{S}^{+})^{+} \quad \leftarrow \text{ordering is reversed}$$
$$= \hat{S}^{+}\hat{H}^{+}\hat{S} \quad \leftarrow \hat{H} = \hat{H}^{+}$$
$$= \hat{S}^{+}\hat{H}\hat{S} \quad \leftarrow \text{this is just } \hat{H}'$$

so,

$$\hat{H}'^{+} = \hat{H}'$$

3) Unitary matrices in the "old" basis remain unitary in the new basis

Let $\hat{U}$ be Hermitian in the "old" basis

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

Let us calculate the inverse

$$\left[\hat{U}' = \hat{S}^{-1}\hat{U}\hat{S}\right]^{-1}$$
$$\hat{U}'^{-1} = \hat{S}^{-1}\hat{U}^{-1}(\hat{S}^{-1})^{-1} \quad \leftarrow \text{ordering is reversed due to cofactor transpose in the inverse}$$
$$\hat{U}'^{-1} = \hat{S}^{-1}\hat{U}^{-1}\hat{S}$$

Now, since $\hat{S}$ is unitary, then $\hat{U}' = \hat{S}^{+}\hat{U}\hat{S}$.

$$\left[\hat{U}' = \hat{S}^{+}\hat{U}\hat{S}\right]^{+}$$
$$\hat{U}'^{+} = \hat{S}^{+}\hat{U}^{+}(\hat{S}^{+})^{+} \quad \leftarrow \hat{S} \text{ and } \hat{U} \text{ are unitary}$$
$$= \hat{S}^{-1}\hat{U}^{-1}\hat{S} \quad \leftarrow \text{we recognize this as } \hat{U}'^{-1}$$
$$\hat{U}'^{+} = \hat{U}'^{-1}$$

Q3. Practice your matrix multiplication.

a) If $\hat{A}$ is a normal matrix, will it remain normal under a unitary similarity transformation?

b) Let $\hat{A}$ and $\hat{B}$ be two commuting matrices in the "old" basis. Will their transformed version $\hat{A}'$ & $\hat{B}'$ remain commuting under a unitary similarity transformation?

Diagonalization

- Choosing a new basis to make a given matrix diagonal.

Given a matrix $\hat{\mathcal{U}}$ we solve the eigenvalue problem.

$$\hat{\mathcal{U}}|\hat{\mu}_n\rangle = \lambda_n|\hat{\mu}_n\rangle.$$

We usually start in the primitive basis.

So, $|\mu_n\rangle$ is a column matrix of the components of the vector $\vec{\mu}_n$ in the primitive basis.

* If $\hat{\mathcal{U}}$ is not yet diagonal in the old (primitive) basis then we construct the similarity matrix:

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

* From the primitive basis, the $\hat{S}$ that we need to diagonalize $\hat{\mathcal{U}}$ is

$$\hat{S} = \left(|\hat{\mu}_1\rangle\ |\hat{\mu}_2\rangle\ \cdots\ |\hat{\mu}_N\rangle\right)$$

↑ column matrix

* When $\hat{\mathcal{U}}$ is also a normal matrix, then

$$\langle\mu_m|\mu_n\rangle = \delta_{mn}$$

and $\hat{S}$ is also unitary.

To demonstrate this, let us obtain $\hat{S}^{+}\hat{S}$

$$\hat{S}^{+}\hat{S} = \begin{pmatrix} \langle\hat{\mu}_1| \\ \langle\hat{\mu}_2| \\ \vdots \\ \langle\hat{\mu}_N| \end{pmatrix}\left(|\hat{\mu}_1\rangle\ |\hat{\mu}_2\rangle\ \cdots\ |\hat{\mu}_N\rangle\right)$$

$$= \begin{pmatrix} \langle\hat{\mu}_1|\hat{\mu}_1\rangle & \langle\hat{\mu}_1|\hat{\mu}_2\rangle & \cdots & \langle\hat{\mu}_1|\hat{\mu}_N\rangle \\ \langle\mu_2|\hat{\mu}_1\rangle & \langle\hat{\mu}_2|\hat{\mu}_2\rangle & \cdots & \langle\hat{\mu}_2|\hat{\mu}_N\rangle \\ \vdots & \vdots & & \\ \langle\mu_N|\hat{\mu}_1\rangle & \langle\mu_N|\hat{\mu}_2\rangle & \cdots & \langle\hat{\mu}_N|\hat{\mu}_N\rangle \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}$$

$$\hat{S}^{+}\hat{S} = \hat{\mathbb{1}} \quad \text{or} \quad \hat{S}^{-1} = \hat{S}^{+}$$

* The transformed $\hat{\mathcal{U}}$ is now diagonal

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

We can show this

$$\hat{\mathcal{U}}' = \hat{S}^{+}\hat{\mathcal{U}}\left(|\mu_1\rangle\ |\mu_2\rangle\ \cdots\ |\mu_N\rangle\right)$$
$$= \hat{S}^{+}\left(\lambda_1|\mu_1\rangle\ \lambda_2|\mu_2\rangle\ \cdots\ \lambda_N|\mu_N\rangle\right)$$
$$= \begin{pmatrix} \langle\mu_1| \\ \langle\mu_2| \\ \vdots \\ \langle\mu_N| \end{pmatrix}\left(\lambda_1|\mu_1\rangle\ \lambda_2|\mu_2\rangle\ \cdots\ \lambda_N|\mu_N\rangle\right)$$

$$\hat{\mathcal{U}}' = \begin{pmatrix} \lambda_1\langle\hat{\mu}_1|\hat{\mu}_1\rangle & \lambda_2\langle\hat{\mu}_1|\hat{\mu}_2\rangle & \cdots & \lambda_N\langle\hat{\mu}_1|\hat{\mu}_N\rangle \\ \lambda_1\langle\mu_2|\hat{\mu}_1\rangle & \lambda_2\langle\hat{\mu}_2|\hat{\mu}_2\rangle & \cdots & \lambda_N\langle\hat{\mu}_2|\hat{\mu}_N\rangle \\ \vdots & \vdots & & \\ \lambda_1\langle\mu_N|\hat{\mu}_1\rangle & \lambda_2\langle\mu_N|\hat{\mu}_2\rangle & \cdots & \lambda_N\langle\hat{\mu}_N|\hat{\mu}_N\rangle \end{pmatrix}$$

$$= \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \\ 0 & 0 & & \lambda_N \end{pmatrix}$$

Example: Consider the Hermitian matrix

$$\hat{H} = \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix}$$

For eigenvalue $\lambda = 4$ For eigenvalue $\lambda = -2$

$$|x_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \qquad |x_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \qquad |x_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

The similarity transformation is

$$\hat{S} = \left(|x_1\rangle\ |x_2\rangle\ |x_3\rangle\right) = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

Since $\hat{H}$ is Hermitian, then $\hat{S}$ is unitary

$$\hat{S}^{+} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}$$

Calculate $\hat{H}'$

$$\hat{H}' = \hat{S}^{+}\hat{H}\hat{S}$$
$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$
$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} \frac{4}{\sqrt{2}} & -\frac{2}{\sqrt{2}} & 0 \\ 0 & 0 & -2 \\ \frac{4}{\sqrt{2}} & \frac{2}{\sqrt{2}} & 0 \end{pmatrix}$$

$$\hat{H}' = \begin{pmatrix} 4 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

Note that $\hat{H}'$ has the same set of eigenvalues as $\hat{H}$ but different eigenvectors

for eigenvalue $\lambda = 4$ for eigenvalue $\lambda = -2$

$$|x_1'\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |x_2'\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},\quad |x_3'\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Q4. Diagonalize the matrix

$$\hat{M} = \begin{pmatrix} 1 & i\sqrt{8} & 0 & 0 \\ -i\sqrt{8} & 1 & i\sqrt{8} & 0 \\ 0 & -i\sqrt{8} & 1 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

a) Show the similarity transformation $\hat{S}$.

b) Is $\hat{S}$ unitary?