# Lecture 8: Simultaneous Diagonalization

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# Motivation in Quantum Physics

- Physical observables of interest are energy $\boldsymbol{H}$, spin $\boldsymbol{\sigma}$ etc.
- These observables are denoted by Hermitian operators
- Observables are measured simultaneously only in a shared eigenbasis
- Need to diagonalize their corresponding Hermitian operators!

# Simultaneous Diagonalization of Hermitian Operators

For some Hermitian $\boldsymbol{A}$ and $\boldsymbol{B}$, there exists a unitary $\boldsymbol{U}$, such that

$$\boldsymbol{U}^\dagger \boldsymbol{A}\boldsymbol{U} = \boldsymbol{A}_\mathrm{D} \quad \text{and} \quad \boldsymbol{U}^\dagger \boldsymbol{B}\boldsymbol{U} = \boldsymbol{B}_\mathrm{D}$$

$$\text{iff } [\boldsymbol{A}, \boldsymbol{B}] = 0$$

Proof

Let a unitary $\boldsymbol{U}$ transform the operator $\boldsymbol{A}$ to its eigenbasis

$$\mathbb{V}_\mathbb{A} = \{|v_1\rangle, |v_2\rangle, |v_3\rangle \ldots |v_N\rangle\}$$

$\boldsymbol{A}$ must be diagonal in $\mathbb{V}_\mathbb{A}$

$$\boldsymbol{A}_\mathrm{D} = \begin{bmatrix} \alpha_1 & 0 & \ldots \\ 0 & \alpha_2 & \ldots \\ \vdots & \vdots & \ddots \end{bmatrix} \quad \text{with eigenvalues } \alpha_i$$

Note the commutator will not change,

$$(\boldsymbol{U}^\dagger \boldsymbol{A}\boldsymbol{U})(\boldsymbol{U}^\dagger \boldsymbol{B}\boldsymbol{U}) - (\boldsymbol{U}^\dagger \boldsymbol{B}\boldsymbol{U})(\boldsymbol{U}^\dagger \boldsymbol{A}\boldsymbol{U}) = \boldsymbol{U}^\dagger[\boldsymbol{A}, \boldsymbol{B}]\boldsymbol{U} = 0$$

# What happens to $\boldsymbol{B}$ in $\mathbb{V}_A$?

To answer this, lets look at the elements of the commutator in $\mathbb{V}_A$

$$
\begin{aligned}
0 &= [(\boldsymbol{U}^\dagger \boldsymbol{A} \boldsymbol{U}), (\boldsymbol{U}^\dagger \boldsymbol{B} \boldsymbol{U})]_{ij} \\
&= [\boldsymbol{A}_\mathrm{D}, \boldsymbol{B}']_{ij} \\
&= (\boldsymbol{A}_\mathrm{D} \boldsymbol{B}')_{ij} - (\boldsymbol{B}' \boldsymbol{A}_\mathrm{D})_{ij} \\
&= \sum_k \boldsymbol{A}_{\mathrm{D}\,ik} \boldsymbol{B}'_{kj} - \sum_l \boldsymbol{B}'_{il} \boldsymbol{A}_{\mathrm{D}\,lj} \\
&= \alpha_i \boldsymbol{B}'_{ij} - \boldsymbol{B}'_{ij} \alpha_j \qquad \ldots \boldsymbol{A}_{\mathrm{D}\,ik} = \alpha_i \delta_{ik} \\
&= (\alpha_i - \alpha_j) \boldsymbol{B}'_{ij}
\end{aligned}
$$

yielding $\boldsymbol{B}'_{ij} = 0$ (diagonal $\boldsymbol{B}'$), provided all $\alpha_i$ are <u>distinct</u>

$$
\boxed{\boldsymbol{U}^\dagger \boldsymbol{A} \boldsymbol{U} = \boldsymbol{A}_\mathrm{D} \quad \text{and} \quad \boldsymbol{U}^\dagger \boldsymbol{B} \boldsymbol{U} = \boldsymbol{B}_\mathrm{D}}
$$

# Handling Repeated Eigenvalues

Suppose $\alpha_1 = \alpha_2$, then we have $\boldsymbol{B}'_{12} \neq 0$. Therefore,

$$\boldsymbol{B}' = \begin{bmatrix} \boldsymbol{B}'_{11} & \boldsymbol{B}'_{12} & 0 & 0 & \dots \\ \boldsymbol{B}'^{*}_{12} & \boldsymbol{B}'_{22} & 0 & 0 & \dots \\ 0 & 0 & \beta_3 & 0 & \dots \\ 0 & 0 & 0 & \beta_4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad \dots \text{ (partially diagonal)}$$

Transform further to a new basis, $\mathbb{F} = \{\underbrace{|v'_1\rangle, |v'_2\rangle}_{\text{new}}, \underbrace{|v_3\rangle \dots |v_N\rangle}_{\text{unchanged}}\}$

where the new eigenkets of $\boldsymbol{B}$,

$$\begin{aligned} |v'_1\rangle &= \tilde{\boldsymbol{P}}_{11} |v_1\rangle + \tilde{\boldsymbol{P}}_{21} |v_2\rangle \\ |v'_2\rangle &= \tilde{\boldsymbol{P}}_{12} |v_1\rangle + \tilde{\boldsymbol{P}}_{22} |v_2\rangle \end{aligned}$$

are taken as linear combinations of the degenerate $|v_1\rangle$ and $|v_2\rangle$

# Diagonalizes the upper-left block of $B'$

With the unitary $\tilde{\boldsymbol{P}}$ ($\tilde{\boldsymbol{P}}_{ij} = \langle v_i | v'_j \rangle$) , we have

$$\tilde{\boldsymbol{P}}^\dagger \underbrace{\begin{bmatrix} \boldsymbol{B}'_{11} & \boldsymbol{B}'_{12} \\ \boldsymbol{B}'^{*}_{12} & \boldsymbol{B}'_{22} \end{bmatrix}}_{2\times 2 \text{ block}} \tilde{\boldsymbol{P}} = \begin{bmatrix} \beta_1 & 0 \\ 0 & \beta_2 \end{bmatrix}$$

Hence the unitary $\boldsymbol{P} = \begin{bmatrix} \tilde{\boldsymbol{P}}_{11} & \tilde{\boldsymbol{P}}_{12} & 0 & 0 & \dots \\ \tilde{\boldsymbol{P}}_{21} & \tilde{\boldsymbol{P}}_{22} & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \begin{bmatrix} \tilde{\boldsymbol{P}} & 0 \\ 0 & \boldsymbol{I} \end{bmatrix}$

will diagonalize $\boldsymbol{B}'$, i.e, $\boxed{\boldsymbol{P}^\dagger \boldsymbol{B}' \boldsymbol{P} = \boldsymbol{B}_{\text{D}}}$

Note that, $\boxed{\boldsymbol{P}^\dagger \boldsymbol{A}_{\text{D}} \boldsymbol{P} = \boldsymbol{A}_{\text{D}}}$ since $\alpha_1 = \alpha_2$

# Compiling

We observe that

$$\boldsymbol{B}_{\mathrm{D}} = \boldsymbol{P}^{\dagger}\boldsymbol{B}'\boldsymbol{P} = \boldsymbol{P}^{\dagger}(\boldsymbol{U}^{\dagger}\boldsymbol{B}\boldsymbol{U})\boldsymbol{P} = (\boldsymbol{U}\boldsymbol{P})^{\dagger}\boldsymbol{B}(\boldsymbol{U}\boldsymbol{P})$$

$$\boldsymbol{A}_{\mathrm{D}} = \boldsymbol{P}^{\dagger}\boldsymbol{A}_{\mathrm{D}}\boldsymbol{P} = \boldsymbol{P}^{\dagger}(\boldsymbol{U}^{\dagger}\boldsymbol{A}\boldsymbol{U})\boldsymbol{P} = (\boldsymbol{U}\boldsymbol{P})^{\dagger}\boldsymbol{A}(\boldsymbol{U}\boldsymbol{P})$$

The unitary $\boldsymbol{UP}$ simultaneously diagonalizes both $\boldsymbol{A}$ and $\boldsymbol{B}$

# Problem

**Q.** In the standard basis, $\mathbb{B} = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$, consider two operators $\boldsymbol{A}$ and $\boldsymbol{B}$ with the following matrix presentations,

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \text{ and } \boldsymbol{B} = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{bmatrix}$$

Find a transform that simultaneously diagonalizes both $\boldsymbol{A}$ and $\boldsymbol{B}$.

**Solution**

First check if they commute

$$\boldsymbol{AB} = \begin{bmatrix} 1 & 0 & -1 \\ 3 & 0 & 3 \\ 1 & 0 & -1 \end{bmatrix} \neq \begin{bmatrix} 1 & 3 & 1 \\ 0 & 0 & 0 \\ -1 & 3 & -1 \end{bmatrix} = \boldsymbol{BA}$$

As discussed, $\boldsymbol{A}$ and $\boldsymbol{B}$ cannot be simultaneously diagonalized