Simultaneous diagonalization of two commuting matrices

Suppose A and B are two diagonalizable matrices that satisfy AB = BA. Then, it can be shown that there exist basis such that both A and B are diagonal. In other words, they are "simultaneously diagonalizable." This fact will turn out to be useful when we talk about the allowed energy of hydrogen atom. Let's first prove this fact in the case that there is at most one eigenstate with a given eigenvalue.

Let $|\psi_{\lambda_A}\rangle$ satisfy

$$A|\psi_{\lambda_A}\rangle = \lambda_A |\psi_{\lambda_a}\rangle \tag{1}$$

Then,

$$AB|\psi_{\lambda_A}\rangle = BA|\psi_{\lambda_A}\rangle \tag{2}$$

$$AB|\psi_{\lambda_A}\rangle = B\lambda_A|\psi_{\lambda_A}\rangle \tag{3}$$

$$A(B|\psi_{\lambda_A}\rangle) = \lambda_A(B|\psi_{\lambda_A}\rangle) \tag{4}$$

Thus, $B|\psi_{\lambda_A}\rangle$ is also an eigenstate of A with the eigenvalue λ_A . Since there is at most one eigenvector for a given eigenvalue, this state must be proportional to $|\psi_{\lambda_A}\rangle$. Thus, we can write

$$B|\psi_{\lambda_A}\rangle = \lambda_B|\psi_{\lambda_A}\rangle \tag{5}$$

for some λ_B . Now, notice that this is an eigenvalue equation for the matrix B! We see that $|\psi_{\lambda_A}\rangle$ is not only an eigenvector of A, but also an eigenvector for B. Thus, if we take the eigenvector of A as the basis to represent the matrix A, not only A but also B is diagonal.

Now, let's consider the case when there is more than one eigenvector for a given eigenvalue. Let's say there are n independent eigenvectors for the eigenvalue λ_A . Then, (1) becomes

$$A|\psi^{i}_{\lambda_{A}}\rangle = \lambda_{A}|\psi^{i}_{\lambda_{A}}\rangle \tag{6}$$

where i runs from 1 to n. Then (2) and (3) can be similarly written and (4) becomes

$$A(B|\psi_{\lambda_A}^i\rangle) = \lambda_A(B|\psi_{\lambda_A}^i\rangle) \tag{7}$$

So, $B|\psi_{\lambda_A}^i\rangle$ is an eigenvector of A with eigenvalue λ_A . Thus, we can express it as a linear combination of $|\psi_{\lambda_A}^j\rangle$. Therefore, we can write

$$B|\psi_{\lambda_A}^i\rangle = \sum_j C_{ij}|\psi_{\lambda_A}^j\rangle \tag{8}$$

for some C_{ij} . Now, notice that C_{ij} is just the matrix elements of B in the subspace (i.e. subregion) of whole vector space in which B acts on. This subspace is *n*-dimensional. Since B is diagonalizable, C_{ij} must be also diagonalizable. Thus, we conclude the proof.

Summary

• When two diagonalizable matrices commute, it is possible to find a set of common basis on which both of them are diagonal.