SIMULTANEOUS DIAGONALIZATION OF HERMITIAN MATRICES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.10.

The spectral theorem guarantees that any normal operator can be unitarily diagonalized. For commuting hermitian operators we can go one step further and show that a set of such operators can be simultaneously diagonalized with a single unitary transformation. The proof is a bit lengthy and is spelled out in full both in Zwiebach's notes (chapter 6) and in Shankar's book (chapter 1, theorem 13) so I won't reproduce it in full here. To summarize the main points:

We can start by considering two operators Ω and Λ and assume that at least one of them, say Ω, is nondegenerate, that is, for each eigenvalue there is only one eigenvector (up to multiplication by a scalar). Then for one eigenvalue ω_i of Ω we have

$$\Omega\left|\omega_i\right\rangle = \omega_i\left|\omega_i\right\rangle \tag{1}$$

We also have

$$\Lambda\Omega\left|\omega_i\right\rangle = \omega_i\Lambda\left|\omega_i\right\rangle \tag{2}$$

so that, provided $[\Lambda,\Omega]=0$, $\Lambda\left|\omega_i\right\rangle$ is also an eigenvector of Ω for eigenvalue ω_i. However, since Ω is nondegenerate, $\Lambda\left|\omega_i\right\rangle$ must be a multiple of $\left|\omega_i\right\rangle$ so that, we have

$$\Lambda\left|\omega_i\right\rangle = \lambda_i\left|\omega_i\right\rangle \tag{3}$$

so that $\left|\omega_i\right\rangle$ is an eigenvector of Λ for eigenvalue λ_i. Therefore a unitary transformation that diagonalizes Ω will also diagonalize Λ. Note that in this case we didn't need to assume that Λ is nondegenerate.

If both Ω and Λ are degenerate, things are a bit more complicated, but the basic idea is this. Suppose we find a basis that diagonalizes Ω and arrange the basis vectors within the unitary matrix U in an order that groups all equal eigenvalues together, so that all the eigenvectors corresponding to eigenvalue ω_1 occur first, followed by all the eigenvectors corresponding to eigenvalue ω_2 and so on, up to eigenvalue ω_m where $m<n$ is the number

of distinct eigenvalues (which is less than the dimension n of the matrix Ω because Ω is degenerate).

Each subset of eigenvectors corresponding to a single eigenvalue forms a subspace, and we can show that the other matrix Λ, operating on a vector from that subspace transforms the vector to another vector that also lies within the same subspace. Now, any linearly independent selection of basis vectors within the subspace will still diagonalize Ω for that eigenvalue, so we can select such a set of basis vectors within that subspace that also diagonalizes Λ within that subspace. The process can be repeated for each eigenvalue of Ω resulting in a set of basis vectors that diagonalizes both matrices.

Obviously, I've left out the technical details of just how this is done, but you can refer to either Zwiebach's notes or Shankar's book for the details.

As an example, consider the two matrices

$$\Omega = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{4}$$

$$\Lambda = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{bmatrix} \tag{5}$$

We can verify that they commute:

$$\Omega\Lambda = \Lambda\Omega = \begin{bmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{bmatrix} \tag{6}$$

We can find the eigenvalues and eigenvectors of Ω and Λ in the usual way. For Ω we have

$$\det(\Omega - \omega I) = 0 \tag{7}$$

$$(1-\omega)\left[(-\omega(1-\omega))\right] + \omega = 0 \tag{8}$$

$$\omega\left(2\omega - \omega^2\right) = 0 \tag{9}$$

$$\omega = 0, 0, 2 \tag{10}$$

Solving the eigenvector equation, we get, for $\omega = 0$

$$(\Omega - \omega I)\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{11}$$

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{12}$$

$$a = -c \tag{13}$$

$$b = \text{anything} \tag{14}$$

Thus 2 orthonormal eigenvectors are

$$|0_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \tag{15}$$

$$|0_2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{16}$$

For $\omega = 2$:

$$\begin{bmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{17}$$

$$a = c \tag{18}$$

$$b = 0 \tag{19}$$

$$|2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \tag{20}$$

For Λ, we can go through the same procedure to find

$$\det(\Lambda - \lambda I) = 0 \tag{21}$$

$$-\lambda(2-\lambda)^2 + \lambda - 2 + \lambda - 2 - 2 + \lambda = 0 \tag{22}$$

$$(\lambda - 2)[\lambda(2-\lambda) + 3] = 0 \tag{23}$$

$$\lambda = -1, 2, 3 \tag{24}$$

We could calculate the eigenvectors from scratch, but from the simultaneous diagonalization theorem, we know that the eigenvector $|2\rangle$ from Ω must be an eigenvector of Λ, and we find by direct calculation that

$$\Lambda|2\rangle = 3|2\rangle \tag{25}$$

so $|2\rangle$ is the eigenvector for $\lambda = 3$.

For the other two eigenvalues of Λ, we know the eigenvectors must be linear combinations of $|0_1\rangle$ and $|0_2\rangle$ from Ω. Such a combination must have form

$$a|0_1\rangle + b|0_2\rangle = \begin{bmatrix} a \\ b \\ -a \end{bmatrix} \tag{26}$$

so we must have

$$\Lambda \begin{bmatrix} a \\ b \\ -a \end{bmatrix} = \begin{bmatrix} a+b \\ 2a \\ -a-b \end{bmatrix} = \lambda \begin{bmatrix} a \\ b \\ -a \end{bmatrix} \tag{27}$$

for $\lambda = -1, 2$. For $\lambda = 2$, we have

$$a = b \tag{28}$$

$$|\lambda = 2\rangle = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \tag{29}$$

For $\lambda = -1$:

$$b = -2a \tag{30}$$

$$|\lambda = -1\rangle = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ -1 \end{bmatrix} \tag{31}$$

The columns of the unitary transformation matrix are therefore given by 29, 31 and 20, so we have

$$U = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{6}} & 0 \\ -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{32}$$

$$U^\dagger = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{33}$$

By matrix multiplication, we can verify that this transformation diagonalizes both Ω and Λ:

$$U^{\dagger}\Omega U=\left[\begin{array}{ccc}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 2\end{array}\right] \tag{34}$$

$$U^{\dagger}\Lambda U=\left[\begin{array}{ccc}2 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 3\end{array}\right] \tag{35}$$

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