DEGENERATE EIGENVALUES AND GRAM-SCHMIDT ORTHOGONALIZATION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Section 3.2.2; Problem 3.7.

We've seen that for a hermitian operator, there are two important conditions on the eigenvalues and eigenfunctions. First, the eigenvalues of a hermitian operator are real, and correspond to observable properties of a physical system. Second, the eigenfunctions of non-degenerate eigenvalues are orthogonal, possibly with the help of a weighting function.

We'll look now at what happens if two or more solutions of the operator equation have the same eigenvalue, that is, the eigenvalue is *degenerate*. For an operator $\hat{Q}$, we'll look at solutions of

$$\hat{Q}f(x) = qf(x) \tag{1}$$

where there are more than one independent eigenfunction $f(x)$ for the same eigenvalue q.

First, suppose we have two eigenfunctions $f(x)$ and $g(x)$ corresponding to eigenvalue q. Then any linear combination of $f(x)$ and $g(x)$ is also an eigenfunction for the same eigenvalue.

Let $h(x) = Af(x) + Bg(x)$. Then

$$\begin{aligned}
\hat{Q}h(x) &= \hat{Q}(Af(x) + Bg(x)) && (2)\\
&= \hat{Q}Af(x) + \hat{Q}Bg(x) && (3)\\
&= qAf(x) + qBg(x) && (4)\\
&= q(Af(x) + Bg(x)) && (5)\\
&= qh(x) && (6)
\end{aligned}$$

As an example, suppose $\hat{Q} = d^2/dx^2$. Then $f(x) = e^x$ and $g(x) = e^{-x}$ are eigenfunctions with $q = 1$ because $\hat{Q}f(x) = f(x)$ and $\hat{Q}g(x) = g(x)$.

In order to test orthogonality, we need to define an interval over which the solutions apply. Since $f(x)g(x) = 1$ everywhere, it's clear that there is no interval for which these two eigenfunctions are orthogonal. However, there is a method called the Gram-Schmidt method for constructing orthogonal functions that we can use to build a pair of orthonormal (orthogonal and normalized) functions over a given interval.

The procedure is straightforward, although a bit tedious. Suppose we have a set of eigenfunctions $\{f_1, g_1, h_1 \ldots\}$ that is not orthogonal. Then:

1. Normalize f_1 to get the first eigenfunction in the orthonormal set (which will have subscript 2):

$$|f_2\rangle \equiv \frac{|f_1\rangle}{\langle f_1|f_1\rangle^{1/2}} \tag{7}$$

where we're using the bra-ket notation to make things easier.

Next, we find the projection of $|g_1\rangle$ onto $|f_2\rangle$. Remember that the inner product is a generalization of the dot product with three-dimensional vectors, so this projection is

$$\langle f_2|g_1\rangle |f_2\rangle \tag{8}$$

Remember that $|f_2\rangle$ is normalized so its magnitude is 1. We now subtract this projection from $|g_1\rangle$ to get an intermediate vector $|\gamma_2\rangle$:

$$|\gamma_2\rangle \equiv |g_1\rangle - \langle f_2|g_1\rangle |f_2\rangle \tag{9}$$

Note that $|\gamma_2\rangle$ is now orthogonal to $|f_2\rangle$:

$$\begin{aligned} \langle f_2|\gamma_2\rangle &= \langle f_2|g_1\rangle - \langle f_2|g_1\rangle \langle f_2|f_2\rangle && (10)\\ &= \langle f_2|g_1\rangle - \langle f_2|g_1\rangle && (11)\\ &= 0 && (12) \end{aligned}$$

since $\langle f_2|f_2\rangle = 1$.

Ordinarily, $|\gamma_2\rangle$ is not normalized, but this is easily done in principle, and we get the second vector in our orthonormal basis:

$$|g_2\rangle \equiv \frac{|\gamma_2\rangle}{\langle \gamma_2|\gamma_2\rangle^{1/2}} \tag{13}$$

We can continue this way for as many vectors as we need. The next step subtracts the projection of $|h_1\rangle$ onto $|f_2\rangle$ and $|g_2\rangle$ and normalizes the result. That is, we calculate the intermediate vector $|\eta_2\rangle$:

$$|\eta_2\rangle = |h_1\rangle - \langle f_2|h_1\rangle |f_2\rangle - \langle g_2|h_1\rangle |g_2\rangle \tag{14}$$

and normalize it to get $|h_2\rangle$.

Returning to our example above, we can use Gram-Schmidt to produce a pair of orthonormal eigenfunctions. We begin with the basis of $f_1(x) = e^x$ and $g_1(x) = e^{-x}$. Then stage 1 is to normalize f_1 to get f_2:

$$
\begin{aligned}
f_2 &= \frac{|f_1\rangle}{\langle f_1|f_1\rangle^{1/2}} && (15)\\
&= \frac{e^x}{\sqrt{\int_{-1}^1 e^{2x}dx}} && (16)\\
&= \frac{2e^x}{\sqrt{2(e^2-e^{-2})}} && (17)
\end{aligned}
$$

This is the first function in the orthonormal basis. To get the other, we need to evaluate $g_1 - \langle f_2|g_1\rangle|f_2\rangle$ and then normalize it. We find:

$$
\begin{aligned}
\langle f_2|g_1\rangle &= \frac{2}{\sqrt{2(e^2-e^{-2})}}\int_{-1}^1 e^x e^{-x}dx && (18)\\
&= \frac{4}{\sqrt{2(e^2-e^{-2})}} && (19)
\end{aligned}
$$

So:

$$
g_1 - \langle f_2|g_1\rangle|f_2\rangle = e^{-x} - \frac{8e^x}{2(e^2-e^{-2})} \tag{20}
$$

This function is orthogonal to f_2, but we can normalize it to get an orthonormal basis. This gives:

$$
g_2 = \frac{\sqrt{2}e^3}{\sqrt{(e^8-18e^4+1)(e^4-1)}}(4e^x + (e^2-e^{-2})e^{-x}) \tag{21}
$$

It can be verified by direct calculation (using Maple) that $\langle f_2|g_2\rangle = 0$ and that $\langle f_2|f_2\rangle = \langle g_2|g_2\rangle = 1$.

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