

## 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

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

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

$$(2) \quad \hat{Q}h(x) = \hat{Q}(Af(x) + Bg(x))$$

$$(3) \quad = \hat{Q}Af(x) + \hat{Q}Bg(x)$$

$$(4) \quad = qAf(x) + qBg(x)$$

$$(5) \quad = q(Af(x) + Bg(x))$$

$$(6) \quad = qh(x)$$

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  $\{f_1, g_1, h_1 \dots\}$  that is not orthogonal. Then:

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

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

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

$$(8) \quad \langle f_2|g_1\rangle |f_2\rangle$$

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  $|\gamma_2\rangle$ :

$$(9) \quad |\gamma_2\rangle \equiv |g_1\rangle - \langle f_2|g_1\rangle |f_2\rangle$$

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

$$(10) \quad \langle f_2|\gamma_2\rangle = \langle f_2|g_1\rangle - \langle f_2|g_1\rangle \langle f_2|f_2\rangle$$

$$(11) \quad = \langle f_2|g_1\rangle - \langle f_2|g_1\rangle$$

$$(12) \quad = 0$$

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:

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

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  $|\eta_2\rangle$ :

$$(14) \quad |\eta_2\rangle = |h_1\rangle - \langle f_2|h_1\rangle |f_2\rangle - \langle g_2|h_1\rangle |g_2\rangle$$

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  $f_2$ :

$$(15) \quad f_2 = \frac{|f_1\rangle}{\langle f_1|f_1\rangle^{1/2}}$$

$$(16) \quad = \frac{e^x}{\sqrt{\int_{-1}^1 e^{2x} dx}}$$

$$(17) \quad = \frac{2e^x}{\sqrt{2(e^2 - e^{-2})}}$$

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:

$$(18) \quad \langle f_2|g_1\rangle = \frac{2}{\sqrt{2(e^2 - e^{-2})}} \int_{-1}^1 e^x e^{-x} dx$$

$$(19) \quad = \frac{4}{\sqrt{2(e^2 - e^{-2})}}$$

So:

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

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

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

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

#### PINGBACKS

Pingback: Legendre polynomials: generation by Gram-Schmidt process

Pingback: Orthonormal basis and orthogonal complement