CHEM 3610 Lecture Notes
–On Projections–

Matthew Rowley

Fall 2016

Projection onto a Polynomial Basis

Remember that any function can be represented as a sum of all the functions in a basis set, but each basis set function must be *scaled* by a co-efficient:

$$\Psi = \sum_i c_i \phi_i$$

Our goal is to find the values of d_i so that we can know how much each basis function ϕ_i contributes to the function Ψ. This can also be interpreted as a measure of how *similar* is each basis function to Ψ.

This can be accomplished with the simple integral, which can be called the *overlap* integral:

$$c_i = \langle \phi_i | \Psi \rangle = \int \phi_i^* \Psi d\tau$$

Consider the following basis set. These are now normalized, unlike those I showed you in class. Note that these are orthonormal only over the interval $[-1, 1]$.

$$\phi_0(x) = \frac{1}{\sqrt{2}}, \ \ \phi_1(x) = \sqrt{\frac{3}{2}}x, \ \ \phi_2(x) = \frac{\sqrt{15}}{4}\left(x^2 - \frac{1}{3}\right), \ \ \phi_3(x) = \sqrt{\frac{175}{8}}\left(x^3 - \frac{3}{5}x\right)$$

and the function:

$$F(x) = \sin x + \frac{1}{2}$$
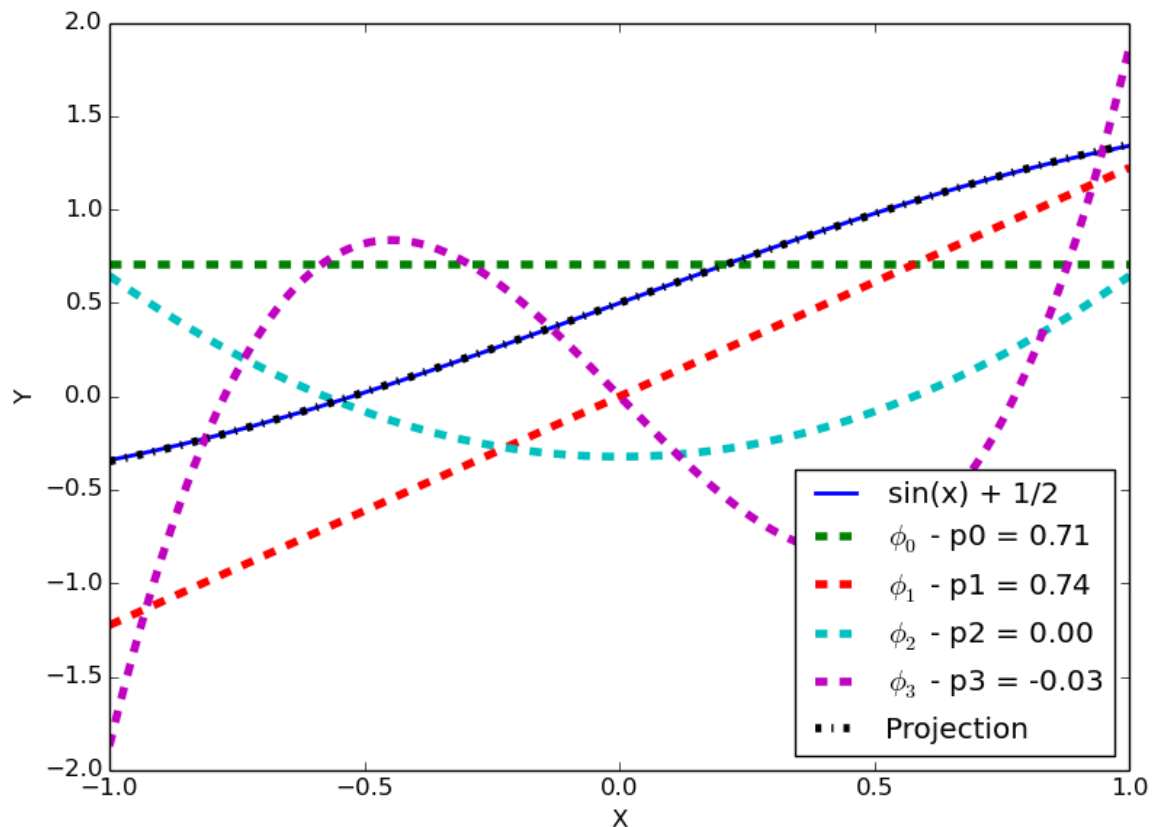
Projecting onto each basis function in turn gives:

$$c_0 = \int_{-1}^{1} \frac{1}{\sqrt{2}} \left(\sin x + \frac{1}{2} \right) dx = \frac{1}{\sqrt{2}} \left[-\cos x + \frac{1}{2}x \right]_{-1}^{1} = \frac{1}{\sqrt{2}}$$

$$c_1 = \int_{-1}^{1} \sqrt{\frac{3}{2}}x \left(\sin x + \frac{1}{2} \right) dx = \sqrt{\frac{3}{2}} \left[\sin x - x \cos x + \frac{1}{4}x^2 \right]_{-1}^{1} = \sqrt{6}\left(\sin(1) - \cos(1) \right)$$

$$c_2 = \int_{-1}^{1} \frac{\sqrt{15}}{4} \left(x^2 - \frac{1}{3} \right) \left(\sin x + \frac{1}{2} \right) dx = 0 \ (exactly)$$

$$c_3 = \int_{-1}^{1} \sqrt{\frac{175}{8}} \left(x^3 - \frac{3}{5}x \right) \left(\sin x + \frac{1}{2} \right) dx = \sqrt{14}\left(14 \cos(1) - 9 \sin(1) \right)$$

The last two I did using Wolfram Alpha because the integrals do get pretty dicey. Below is a figure showing the results (the coefficients are approximate, since I found them numerically).

Projection onto a Fourier Series

Problem P2.32 asks to project the function:

$$f(y) = y^2$$

onto a Fourier series basis set. In other words, find the coefficients for the following equation:

$$f(y) = d_0 + \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi y}{a}\right) + d_n \cos\left(\frac{n\pi y}{a}\right)$$

We see that this Fourier series is a basis set consisting of three types of functions: $d_0 \dfrac{1}{\sqrt{2a}}, c_n \dfrac{1}{\sqrt{a}}\sin\left(\dfrac{n\pi y}{a}\right)$, and $d_n \dfrac{1}{\sqrt{a}}\cos\left(\dfrac{n\pi y}{a}\right)$. Here I have strayed a bit from the derivation in class by normalizing these basis functions up front.

Now we can find the coefficients by doing the same overlap integral as before, namely:

$$c_i = \langle \phi_i | \Psi \rangle = \int \phi_i^* \Psi d\tau$$

Now, we can use symmetry to simplify a few of these. We know that $f(x) = y^2$ is a function with *even* symmetry, while $\sin\left(\dfrac{n\pi y}{a}\right)$ has *odd* (or *antisymmetric*) symmetry. The overlap integral of a product of an even and an odd function will always be 0. We would say that they are orthogonal by symmetry. So, we know that all coefficients c_n are 0.

To get the others, we must perform the integration:

$$d_0 = \int_{-a}^{a} \frac{1}{\sqrt{2a}} y^2 dy = \frac{1}{\sqrt{2a}}\left[\frac{1}{3}y^3\right]_{-a}^{a} = \frac{2\sqrt{2}}{6}a^{5/2}$$

$$d_{n>0} = \frac{1}{\sqrt{a}}\int_{-a}^{a} y^2 \cos\left(\frac{n\pi y}{a}\right) dy$$

$$= \frac{1}{\sqrt{a}}\left[\left(\frac{a}{n\pi}\right)^3\left(\left(\frac{n\pi}{a}\right)^2 y^2 - 2\right)\sin\left(\frac{n\pi y}{a}\right) + \left(\frac{a}{n\pi}\right)^3 2y\cos\left(\frac{n\pi y}{a}\right)\right]_{-a}^{a}$$

$$= \frac{1}{\sqrt{a}}\left[\frac{a}{n\pi}y^2\sin\left(\frac{n\pi y}{a}\right) - \left(\frac{a}{n\pi}\right)^3 2\sin\left(\frac{n\pi y}{a}\right) + \left(\frac{a}{n\pi}\right)^2 2y\cos\left(\frac{n\pi y}{a}\right)\right]_{-a}^{a}$$

Here I made a small mistake in class, so ignore your notes and instead follow what I do now. If your functions are symmetric (or antisymmetric) over your interval, then you can simplify some integrals. An

odd function will integrate to zero, because any positive area will perfectly match a negative area on the other side. Consider finding the area under $f(x) = \sin(x)$ over the interval of $[-\pi, \pi]$ — it will be zero for this reason.

Similarly, an even function will evaluate to zero over the interval because you end up subtracting a value from itself. Here consider evaluating $f(x) = \cos(x)$ over the interval of $[-\pi, \pi]$. You would get $-1 - (-1) = 0$

Remember also the rule: odd x odd = even, even x even = even. and odd x even = odd. This applies to the symmetry of functions as well as to the parity of numbers.

Unfortunately, all of the functions we are evaluating here are odd, so there is no simplification to be done except by evaluating over the interval. Fortunately, $\sin\left(\dfrac{n\pi y}{a}\right)$ still *does* go to zero over the interval $[-a, a]$, just not for reasons of symmetry.

$$
\begin{aligned}
d_{n>0} &= \frac{1}{a}\left[\frac{a}{n\pi}y^2\sin\left(\frac{n\pi y}{a}\right) - \left(\frac{a}{n\pi}\right)^3 2\sin\left(\frac{n\pi y}{a}\right) + \left(\frac{a}{n\pi}\right)^2 2y\cos\left(\frac{n\pi y}{a}\right)\right]_{-a}^{a} \\[2mm]
&= \frac{1}{a}\left[\left(\frac{a}{n\pi}\right)^2 2y\cos\left(\frac{n\pi y}{a}\right)\right]_{-a}^{a} \\[2mm]
&= \frac{1}{\sqrt{a}}\left[\frac{2a^3}{n^2\pi^2}(-1) - \frac{-2a^3}{n^2\pi^2}(-1)\right] = -\frac{4a^{5/2}}{n^2\pi^2} \; for \; odd \; n \\[2mm]
&= \frac{1}{\sqrt{a}}\left[\frac{2a^3}{n^2\pi^2}(1) - \frac{-2a^3}{n^2\pi^2}(1)\right] = \frac{4a^{5/2}}{n^2\pi^2} \; for \; even \; n \\[2mm]
&= (-1)^n \frac{4a^{5/2}}{n^2\pi^2}
\end{aligned}
$$

But wait, a negative coefficient…is that even a thing? Yes, it is very much a thing. Consider the curvature of cosine functions compared to the curvature of y^2. Cosines curve downward while y^2 curves upward, so we have to use the negatives of the cosine functions.

Finally, below is a plot showing how this works, for the case where $a = \pi$.
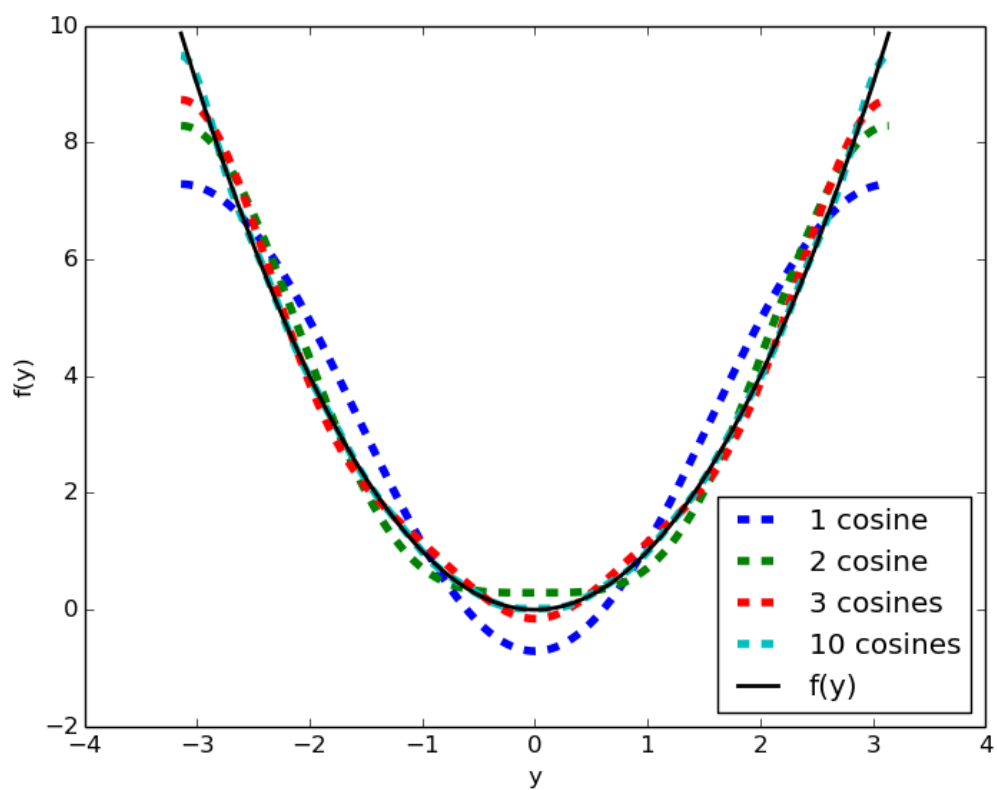
Exam 1 Study Guide

Here is a brief overview of what you need to know for this exam:

- ○ Early quantum experiments, such as:

  - · The spectrum of blackbody radiation

  - · The photoelectric effect

  - · Hydrogen atom emission lines

  - · Single photon diffraction

  - · Matter wave diffraction

- ○ DeBroglie Wavelengths

- ○ Diffraction fringe spacing for given parameters

- ○ Energy level occupancy and the Boltzmann distribution

- ○ Dealing with complex numbers

- ○ Spherical and Cartesian coordinate systems

- ○ Operators in linear algebra

- ○ Eigenfunctions and Eigenvalues

- ○ Normalization of a function

- ○ Orthogonality of functions

- ○ Projection onto a basis set

On the following pages are the equations and formulas which will be provided to you for use during the exam.