Additional: Quick discussion of Fourier Analysis

Here we want to concentrate not primarily on Fourier Analysis but expansions of functions in complete orthonormal functions in general.

First, review vectors

Recall the discussion of vectors and vector spaces. Vectors within a vector space can be represented by an expansion into perpendicular directions. As long as a set of unit vectors is defined that span the space. The unit vectors are an *orthonormal, complete set of vectors*. Complete means that any vector within the space can be represented in the expansion. Thus, for normal spaces, the number of unit vectors is equal to the dimension of the space.

The inner product (dot product) gave us how to find lengths of vectors and angles between vectors (the inner product is a representation of the metric in the space). Thus if we have an n-dimensional space the inner products of any vector can be broken down into the inner products of the basis vectors,

$$\begin{aligned} \langle i|j\rangle &= 0 \qquad \text{for } i \neq j \qquad \text{ortho} \\ \langle i|i\rangle &= 1 \qquad \text{for } i = 1, 2, ...n. \qquad \text{normal} \end{aligned}$$

These two conditions can be more compactly expressed in terms of the *Kronecker delta*, δ_{ij} which has the simple property of being 1 when $i = j$ and 0 when $i \neq j$. Thus the orthonormal condition is expressed as,

$$\langle i|j\rangle = \delta_{ij}$$

Any vector in this vector space can then be expressed as,

$$|V\rangle = a_1|1\rangle + a_2|2\rangle + a_3|3\rangle + \cdots + a_n|n\rangle = \sum_{i=1}^{n} a_i|i\rangle$$

If you want to find any of the components of this vector, for e.g. you are asked 'what is the extent of this vector in the 27^{th} dimension?', you simply use the inner product,

$$\langle 27|V\rangle = \langle 27|a_{27}|27\rangle = a_{27}$$

all the other inner products vanishing due to the orthogonality of the basis vectors. This general idea is behind the expansion of functions in an orthonormal, complete basis of *functions* that we look at next.

1 Expansion in terms of harmonic functions

We will start with a simple example, the space of periodic functions on the circle (S^1). In this case there is one parameter θ that maps out all points. However now we are not concerned about mapping locations within this space but the set of periodic functions that can exist. If you think about you can have a wildly fluctuating function here that looks random and all we ask is that it comes back to itself when $\theta \to \theta 2\pi$. We want a method to represent these functions in a simpler manner.

In analogy to the vector case, we want to define a basis that is orthonormal and complete. Then we can expand our complicated function in terms of this basis.

Thus, I propose we look at the following function,

$$f_n(\theta) = e^{in\theta} \qquad \text{where, } n = 0, \pm 1, \pm 2, \pm 3, \cdots \pm \infty$$

This is an infinite set of vectors that we can make into an orthonormal, complete basis. First, we need to define the inner product in this function space. Since our basis vectors are complex, we need to complex conjugate the first entry.

$$\langle f|g\rangle = \int_0^{2\pi} f^* g d\theta$$

The left hand side is written in a similar form as for vectors, this is just for notational convenience. I could also define the functions as vectors if I wish ($f(\theta) \to |f\rangle$), perhaps later we might represent them that way.

So again, the inner product in this function space is to conjugate the first entry multiply by the second, and integrate over the space (θ). Let's see if our proposed basis above works. (We will suppress the θ dependence for clarity, $f_n(\theta) \rightarrow f_n$). First, are these functions normalized?

$$\begin{aligned}
\langle f_n | f_n \rangle &= \int_0^{2\pi} f_n^* f_n d\theta \quad = 1? \\
&= \int_0^{2\pi} e^{-in\theta} e^{in\theta} d\theta = \int_0^{2\pi} d\theta = 2\pi.
\end{aligned}$$

Huh, they are not normalized. This is easily remedied by redefining our proposed basis as

$$f_n(\theta) \;=\; \frac{1}{\sqrt{2\pi}} e^{in\theta} \qquad \text{where,}\;\; n = 0, \pm 1, \pm 2, \pm 3, \cdots \pm \infty$$

Now they are normalized. Are they orthogonal?

$$\begin{aligned}
\langle f_n | f_m \rangle &= \frac{1}{2\pi} \int_0^{2\pi} e^{-in\theta} e^{im\theta} d\theta = \frac{1}{2\pi} \int_0^{2\pi} e^{i(m-n)\theta} \quad \text{with} \quad n \neq m \\
&= \frac{1}{2\pi} \left[\frac{1}{i(m-n)} e^{i(m-n)\theta} \right|_0^{2\pi} = \frac{1}{2i\pi(m-n)} \left[e^{i(m-n)2\pi} - 1 \right] = \frac{1}{2i\pi(m-n)} [1-1] = 0
\end{aligned}$$

Thus this basis is orthogonal since $m - n$ is an integer and $e^{in2\pi} \sim \cos(2\pi n) + \sin(2\pi n) = 1$. Thus we have an orthonormal set of vectors. Is the set complete? Well, since we can consider any function with arbitrarily high frequencies we need a basis that can handle it. Thus, if we have an infinite set of basis vectors, as given in our definition (n up to $\pm\infty$), we can handle any frequency. So they are complete. Thus our function space is infinite dimensional.

Ok let's see how this works. Given an arbitrary function $g(\theta)$, it can now be expressed as an infinite sum of components in each dimension of this function space.

$$g(\theta) \;=\; \sum_{j=-\infty}^{+\infty} a_j f_j = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{+\infty} a_j e^{ij\theta} \tag{1}$$

Finding the expansion

Ok, let's say we are given a function $g(\theta)$ and we want to create this expansion (perhaps out to so many terms), how do we do it? Think back to the vectors, to specify this expansion we just need to find the coefficients a_j. We said how to do it for vectors, the same applies here. So let's find the 27^{th} coefficient (calling $g \rightarrow |g\rangle$ for the moment).

$$a_{27} \;=\; \langle 27 | g \rangle = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{-i\,27\,\theta} g(\theta) d\theta$$

Again, this works because the basis functions are orthogonal. The idea is almost exactly the same as with vectors. In fact, many go ahead and write the basis functions as unit vectors and go from there.

Notice also we could have defined other bases that may be more useful. For example, since we are dealing with complex exponentials, I could also have used sines and cosines. That is, define,

$$|n\rangle \;=\; \frac{1}{\sqrt{2\pi}} \cos(n\theta) + \sin(n\theta)$$

where now we do not need to worry about complex conjugating the bra vector when we form our inner product.

We do need to be a little careful to make sure that all of the integrals exist, that the series converges, and does so to the function. We will not worry about these technicalities and assume all is good as we proceed.

General function expansions

Thus the method in the last section can be made more general and thus extended to different types of function spaces.

1) Define the function space. How many independent parameters are there (what dimension functions are we considering)? Are the parameters finite? Periodic (like above)?, Infinite?

2) Define the inner product in this function space.

3) Construct a complete orthonormal basis of functions.

- Expand away!

There are many type of expansions that can be considered.

Example: Legendre Polynomials

An example that arises in electrostatics and quantum mechanics (Hydrogen atom) are functions defined on the line $-1 \leq x \leq +1$. These arise in trying to find solutions for the Laplacian in spherical coordinates (the Θ equation of $\Psi = R\Theta\Phi$) where $x \equiv \cos(\theta)$. Let's break it down.

1) The space of functions are those defined on the line $-1 \leq x \leq +1$. It is not necessarily periodic.

2) The inner product is defined as,

$$\langle g|f\rangle = \int_{-1}^{1} g(x)f(x)dx$$

3) The *Legendre* polynomials, $P_l(x)$, form an *orthogonal* set of functions on this function space. *Note, they are not normalized* this is a convention. The first several are listed in the appendix at the end. The orthogonality condition is expressed as,

$$\int_{-1}^{1} P_{l'}(x)P_l(x)dx = \frac{2}{2l+1}\delta_{l'l}$$

We can easily define an orthonormal set as follows,

$$U_l(x) = \sqrt{\frac{2l+1}{2}}P_l(x)$$

However, just to keep us on our toes, this set is rarely used.

- Any function defined on this interval can be expanded in this infinite basis.

Example: Hermite Polynomials

These are often the first set of orthogonal polynomials one sees in a formal quantum mechanics class. They are the set of solutions for the differential equation that results for Schrödinger equation of a particle in a one dimensional harmonic oscillator potential.

As defined in Park (see page 126).

1) The space of functions is over the real line: $-\infty \leq y \leq \infty$.

2) The inner product is defined as,

$$\langle g|f\rangle = \int_{-\infty}^{\infty} g(x)f(x)dx$$

3) The *Hermite polynomials*, $H_l(y)$, are an orthogonal set of polynomials

$$\int_{-\infty}^{\infty} H_{l'}(y)H_l(y) = N_{l'l}\delta_{l'l}$$

The polynomials are not normalized. If you are interested in how these are used to solve the harmonic oscillator, see section 4.6 and then page 126 of Park.

Example: Spherical Harmonics

Now we go up a dimension and consider a set of functions that are defined on the 2-sphere. These are solutions of the particle on the 2-sphere -the optional question assigned.

1) The functions are over the two angles θ, ϕ where they range over,

$$\phi : [0, 2\pi] \qquad\qquad \theta : [0, \pi]$$

The coordinates are periodic.

2) The inner product is defined as,

$$\langle f|g\rangle \quad = \quad \int_0^{2\pi}\int_0^{\pi} f^*(\theta,\phi)g(\theta,\phi)\sin\theta d\theta d\phi$$

3 The spherical harmonic functions, $Y_l^m(\theta,\phi)$ are comprised of the *associated Legendre polynomials*, $P_l^m(\cos\theta)$ (for the θ portion). The polynomials, $P_l^m(\cos\theta)$ are listed in the appendix.

$$Y_l^m(\theta,\phi) \quad = \quad \epsilon\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta)$$

The factor in front is $\epsilon = (-1)^m$ for $m \geq 0$ and 1 for $m \leq 0$. The full orthonormal relation of these harmonics are,

$$\int_0^{2\pi}\int_0^{\pi}[Y_l^m(\theta,\phi)]^*[Y_{l'}^{m'}(\theta,\phi)]\sin\theta d\theta d\phi = \delta_{ll'}\delta_{mm'}$$

Again, these are solutions to the free particle on a 2-sphere and are also important if you want to interpret the data from the WMAP probe. See `www.nasa.gov/topics/universe/features/wmap_five.html` and the plot attached to the end of this document.

- Any function can be expanded in terms of this basis.

$$g(\theta,\phi) \quad = \quad \sum_{l=1}^{\infty}\sum_{m=-l}^{m=+l} g_{lm}Y_l^m(\theta,\phi)$$

Fourier Analysis

We've already met the most basic aspects of Fourier analysis above. Consider a space of functions over the periodic line $-\pi \leq x \leq +\pi$ (this is identical to our previous case of $0 \leq \theta \leq 2\pi$). We already introduced the orthonormal basis in terms of complex exponentials and sines and cosines. Often the first case treated is in terms of sines and cosines.

$$|n\rangle \quad = \quad \cos(nx) + \sin(nx)$$

(where often the normalization constant is absorbed into the expansion coefficients). Using this basis we can expand a function as,

$$f(x) \quad = \quad \frac{a_0}{2} + \sum_{n=1}^{\infty}[a_n\cos(nx) + \sin(nx)]$$

This is the common way to express what is called a *Fourier series*. The expansion coefficients are determined exactly as before (but now including the normalization constant).

$$\begin{aligned} a_n &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)dx \\ b_n &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(nx)dx \end{aligned} \tag{2}$$

There are several variations of defining the normalization and notation but the basic idea is always the same as what we did above.

Relation to quantum mechanics

Quantum mechanics is intimately tied to Fourier analysis and can be thought simply as an application of it. Recall that for a measurement of a particular observable quantity, we want to express the wavefunction in the appropriate basis if we wish to get the probability distribution for that observable.

Consider position and momentum. We introduced the wavefunction initially in *the position basis*, where x and t were the independent variables and we had the Born probability rule,

$$prob(x,t) \quad = \quad \psi^*(x,t)\psi(x,t)$$

(I am using *prob* to express the probability density to avoid confusion with momentum). We could get expectation values of momentum and other observables in this basis however if we change the experiment and measure the momentum, we want to calculate the probability distribution *in momentum.* Thus, we represent the wave function in the *momentum basis.* To emphasize the difference we used a different Greek letter $\Phi(p,t)$ and now it is p and t that are our independent variables. The Born rule is now,

$$prob(p,t) \quad = \quad \Phi^*(p,t)\Phi(p,t)$$

Now, note that these two functions ψ and Φ are representing the same quantum state. They are the same wavefunction expressed in two different bases.

The question is how do we get one from the other?

Recall our plane wave state (in the position basis).

$$\psi(x,t) \quad = \quad e^{\frac{i}{\hbar}(p_0x-Et)}$$

This was a state of *definite* momentum p_0 (which is a constant here). The probability distribution of the plane wave state in the momentum basis is a Dirac delta function. That is, it is a function that is nonzero at $p = p_0$ and zero everywhere else. It is expressed as, $\delta(p - p_0)$ and is really just the continuous analog of the Kronecker delta. (More formally $\delta(0) = 1, \delta(c) = 0 \;\; if \;\; c \neq 0$). Thus our plane wave state in the momentum basis is,

$$prob(p,t) = \Phi^*(p,t)\Phi(p,t) \quad = \quad \delta(p-p_0)$$

Since the measurement of momentum in this case will return the result p_0 with probability 1, the normalization of probability here gives,

$$1 \quad = \quad \int_{-\infty}^{+\infty} \Phi^*(p,t)\Phi(p,t)dp = \int_{-\infty}^{+\infty} \delta(p-p_o)dp$$

This is the general property of the Dirac delta function. It is is zero everywhere except at one point and zero everywhere else, but the area under its curve is 1. You can think of it as an infinitely tall function that has no width such that the area under it is 1 (think of a limiting form if this is melting your mind).

Now consider the reverse case, where we have localized a particle to one position x_0. In this case, the probability distribution in the position basis is a Dirac delta function,

$$1 \quad = \quad \int_{-\infty}^{+\infty} \psi^*(x,t)\psi(x,t)dx = \delta(x-x_0)$$

And in this case the momentum basis wavefunction is,

$$\Phi(p,t) \quad = \quad e^{\frac{i}{\hbar}(px_0-Et)}$$

Thus these expressions must be related.

Notice that our plane wave state is somewhat similar to our basis functions defined in section 1. We want to try to now create a basis in which to expand our wavefunctions. So,

1) The function space is over the real line, $-\infty \leq x \leq +\infty$, (and time which we will ignore for now).

2) The inner product is defined as,

$$\langle f|g\rangle \quad = \quad \int_{-\infty}^{+\infty} f^* g dx$$

3) We want to try to use our plane wave states (of definite momentum) as an orthonormal basis. Thus, are they normalized?

$$\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}(px-Et))} e^{\frac{i}{\hbar}(px-Et))} dx = \int_{-\infty}^{+\infty} dx = \infty$$

We already explored this before -the plane wave state is not normalizable. Before proceeding, let's examine orthogonality. Are they orthogonal? Here we want to consider plane wave states of different momentum (p is taking the place of n that we used in section 1).

$$\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}(px-Et))} e^{\frac{i}{\hbar}(p'x-Et))} dx = \int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}(p-p')x} dx = 0 \quad if\ p \neq p'$$

The argument is the same as in section 1[1] Thus they are orthogonal but are normalized to infinity.

Note now that if we write the orthonormal relations in terms of the Dirac delta function it will not only appear very similar to our section 1 result, but will give us what we need. That is,

$$\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}(px-Et)} e^{\frac{i}{\hbar}(p'x-Et)} dx = 2\pi\delta(p-p')$$

and we have our orthogonal basis we desire (probably should not call it an ortho*normal* basis since they are normalized to a delta function and not 1). The factor of 2π comes from taking the limit of a finite interval to an infinite line. See Park appendix 3 (page 561) for details.

Notice, this gives us a definition of the Dirac delta function (written in terms of wavenumber instead of momentum),

$$\delta(k-k') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i(k-k')x} dx$$

- Now we can expand any wavefunction on the real line in terms of this basis. I.e.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \Phi(p) e^{\frac{i}{\hbar}(px-Et)} dp$$

  Note that this is a continuous version of the expansion (1), instead of summing over j, we are integrating over p.

Notice that our coefficients are a function of momentum (just as the coefficients in (1) are discrete functions of j). These expansion factors are not a function of time because the plane wave states have constant momentum. This is the key result we want. The function $\Phi(p)$ is exactly the momentum basis representation of this wave function.

This transformation is known as a Fourier transform. We can now freely go back and forth between the position basis and momentum basis,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \Phi(p) e^{\frac{i}{\hbar}(px-Et)} dp$$
$$\Phi(p) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \psi(x,t) e^{-\frac{i}{\hbar}(px-Et)} dx$$

Note though, the full momentum basis wave function is $\Phi(p,t) = \Phi(p)e^{-\frac{i}{\hbar}Et}$.

***More to come but that is most of it.

What does it mean?

I find the easiest way to understand a Fourier transform is with a sound wave. The two complementary bases in this case is the waveform, i.e. the amplitude at each position in space changing in time and the frequency spectrum, i.e. the amplitude at each frequency of sound. Each frequency being represented as a a nice sine wave (the basis function). These complementary ways to think of a sound is analogous to what is going in in QM.

[1] You may not note this immediately but consider chopping up the infinite line into equal segments, each one wavelength of this plane wave, ($\lambda = \frac{h}{p-p'}$). Over each wavelength the integral will vanish. Or better yet, think of the cosine part of the plane wave oscillating over the whole real line. There are equal areas above the axis and below of the cosine function - these cancel each other.

Appendix: Some sets of orthogonal functions

Legendre polynomials

Defined on the interval $-1 \leq x \leq +1$. These *are not* normalized. The condition is,

$$\int_{-1}^{1} P_{l'}(x) P_l(x) dx = \frac{2}{2l+1}\delta) l' l$$

$$\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= \frac{1}{2}(3x^2 - 1) \\
P_3(x) &= \frac{1}{2}(5x^3 - 3x) \\
P_4(x) &= \frac{1}{8}(35x^4 - 30x^2 + 3)
\end{aligned}$$

Hermite polynomials

Defined on the interval $-\infty \leq y \leq +\infty$.

$$\begin{aligned}
H_0(y) &= 1 \\
H_1(y) &= 2y \\
H_2(y) &= 4y^2 - 2 \\
H_3(y) &= 8y^3 - 12y \\
H_4(y) &= 16y^4 - 48y^2 + 12
\end{aligned}$$

associated Legendre polynomials

Defined on the interval $-1 \leq \cos\theta \leq +1$.

$$P_1^1(\cos\theta) = \sin\theta \qquad P_2^2(\cos\theta) = 3\sin^2\theta \qquad P_3^3(\cos\theta) = 15\sin\theta(1-\cos^2\theta)$$

$$P_0^1(\cos\theta) = \cos\theta \qquad P_2^1(\cos\theta) = 3\cos\theta\sin\theta \qquad P_3^2(\cos\theta) = 15\sin^2\theta\cos\theta$$

$$P_2^0(\cos\theta) = \tfrac{1}{2}(3\cos^2\theta - 1) \qquad P_3^1(\cos\theta) = \frac{3}{2}\sin\theta(5\cos^2\theta - 1)$$

$$P_3^0(\cos\theta) = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$$

Appendix: WMAP results

Figure 1: WMAP results of temperature fluctuations as a function of spherical harmonic moments l. See `en.wikipedia.org/wiki/Spherical_harmonics` for a nice picture of the spherical harmonics.