CHEM1030 - Week 24 Lecture - function spaces

Chapter 15 of Steiner, "The Chemistry Maths Book", 2nd edition.

Function spaces in general

The rigorous definition of a space does not require the elements to be vectors – the set only needs to be closed under addition and multiplication by a scalar, as well as satisfy the properties of spaces that were given in the previous lectures. In particular, we can easily demonstrate that the set F of all continuous complex functions is a space, because:

1. The sum of two continuous functions is a continuous function: $\forall f, g \in F \quad (f+g) \in F$.
2. A continuous function times a scalar is a continuous function: $\forall f \in F \quad \forall c \in \mathbb{C} \quad (cf) \in F$.
3. There exists a zero function: $\exists 0 \in F: \quad \forall f \in F \quad f + 0 = f$.
4. Each function has an additive inverse: $\forall f \in F \quad \exists(-f) \in F: \quad f + (-f) = 0$
5. The usual associativity and distributivity laws hold for addition and multiplication by a scalar.

We can use the analogy with vectors and look at the notion of "length" and "scalar product" for functions, as well as at ways of expressing functions as linear combinations of other functions. That would be a generalization of the Taylor series – the terms would no longer be just powers of x.

A function f is called a *linear combination* of functions $\{g_1, g_2, g_3, \ldots\}$ if it can be expressed as

$$f = a_1 g_1 + a_2 g_2 + a_3 g_3 + \ldots \qquad\qquad |f\rangle = a_1 |g_1\rangle + a_2 |g_2\rangle + a_3 |g_3\rangle + \ldots$$

in which $\{a_1, a_2, a_3, \ldots\}$ are some complex numbers. Standard mathematical notation is on the left and the notation used in quantum mechanics is on the right. Expansions of this type are *unique* if none of the functions $\{g_1, g_2, g_3, \ldots\}$ themselves may be expressed as a linear combination of other functions from the same set. More generally, a set of functions is called *linearly independent* if none of the functions can be expressed as a linear combination of other functions from the same set.

Example 1: it is easy to demonstrate that the set of power functions $\{x^0, x^1, x^2, x^3, x^4, \ldots\}$ is linearly independent. This linear independence leads to the uniqueness of Taylor expansions.

A set of functions is called a *basis set* of a space if any function in that space may be expressed as a linear combination of the elements of that set. The set of power functions above is an example of a basis set in a space of all infinitely differentiable functions of x.

Function norm and scalar product

By analogy with vector spaces, we can establish the notions of norm and scalar product in function spaces. There are many ways of doing this, but the way that is most closely aligned with physics is:

$$\|f(x)\| = \sqrt{\int f^*(x) f(x)\, dx} \qquad\qquad \langle f(x) | g(x) \rangle = \int f^*(x) g(x)\, dx$$

where $\|f(x)\|$ is called the *norm* of the function $f(x)$, $\langle f(x) | g(x) \rangle$ is called the *scalar product* of functions $f(x)$ and $g(x)$, the star denotes complex conjugation and the integrals are taken over the part of the real axis that is relevant to the problem at hand, in the most general case from $-\infty$ to ∞. Function norm and scalar product are encountered very often and their definitions must be memorized.

Norms and scalar products of multivariate functions are computed in a similar way, by integrating over all available variables. By its nature, the "length" is a real quantity, therefore the norm of a function is always real and non-negative (only the zero function has a zero norm). Scalar products, however, are in general complex numbers.

Example 2: calculate the norm of $f(x)=2x+ix^2$ on the interval $x\in[0,1]$.
Solution: using the definition of the norm, we obtain

$$\|f(x)\|=\sqrt{\int_0^1 f^*(x)f(x)\,dx}=\sqrt{\int_0^1 \left(2x-ix^2\right)\left(2x+ix^2\right)dx}=\sqrt{\int_0^1 \left(4x^2+x^4\right)dx}=\sqrt{\frac{23}{15}}$$

Example 3: calculate the scalar product of $\cos x$ and $\sin x$ on the interval $x\in[-\pi,\pi]$.
Solution: using the definition of the scalar product, we obtain

$$\langle\cos x|\sin x\rangle=\int_{-\pi}^{\pi}\cos(x)\sin(x)\,dx=\frac{1}{2}\int_{-\pi}^{\pi}\sin(2x)\,dx=0$$

Orthonormal function sets

The set of functions $\{g_1(x),g_2(x),g_3(x),\ldots\}$ such that

$$\|g_k(x)\|=1\quad\forall k\quad\text{and}\quad\langle g_k(x)|g_n(x)\rangle=\delta_{kn},\quad\text{where}\quad\delta_{kn}=\begin{cases}1 & \text{if } k=n\\ 0 & \text{if } k\neq n\end{cases}$$

is called an *orthonormal set* – all functions are mutually orthogonal and every function has a unit norm. This is the function space equivalent of the 2D or 3D coordinate axis direction vectors. If the set $\{g_k(x)\}$ also happens to be the basis set for the space it belongs to (*i.e.* every other function of that space may be expressed as their linear combination), it is called an *orthonormal basis set*.

Example 4: demonstrate that the set of functions $g_n(x)=\cos(nx)/\sqrt{\pi}$, where n is a positive integer, is an orthonormal set on the interval $x\in[-\pi,\pi]$.
Solution: we need to demonstrate the normalization

$$\|g_n(x)\|=\left\|\frac{\cos(nx)}{\sqrt{\pi}}\right\|=\sqrt{\frac{1}{\pi}\int_{-\pi}^{\pi}\cos^2(nx)\,dx}=\sqrt{\frac{1}{2\pi}\int_{-\pi}^{\pi}\left[1-\cos(2nx)\right]dx}=\sqrt{\frac{1}{2\pi}2\pi}=1$$

and the orthogonality for the case when $n\neq k$

$$\langle g_n(x)|g_k(x)\rangle=\frac{1}{\pi}\int_{-\pi}^{\pi}\cos(nx)\cos(kx)\,dx=\frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\cos\left[(n-k)x\right]+\cos\left[(n+k)x\right]\right)dx=\delta_{nk}$$

The symbol δ_{nk} is called *Kronecker symbol*, after Leopold Kronecker.

Orthonormal basis sets provide a simple way to express a function as a linear combination of the functions that make up the set:

$$|f(x)\rangle=a_1|g_1(x)\rangle+a_2|g_2(x)\rangle+a_3|g_3(x)\rangle+\ldots=\sum_{n=1}^{\infty}a_n|g_n(x)\rangle$$

The expression for the coefficients $\{a_1,a_2,a_3,\ldots\}$ is surprisingly easy to find, we only need to calculate the scalar product of both sides with $g_k(x)$. Because the set $\{g_n(x)\}$ is orthonormal, only one term survives on the right hand side:

$$\langle g_k(x)|f(x)\rangle=\sum_{n=1}^{\infty}a_n\langle g_k(x)|g_n(x)\rangle=\sum_{n=1}^{\infty}a_n\delta_{nk}=a_k$$

This leads to a very important conclusion – if a function $f(x)$ belongs to a particular function space and $\{g_n(x)\}$ is an orthonormal basis set of that space, then $f(x)$ may be represented as a linear combination of the functions $\{g_n(x)\}$ as follows:

$$|f(x)\rangle = \sum_{n=1}^{\infty} a_n |g_n(x)\rangle \qquad a_n = \langle g_n(x)|f(x)\rangle$$

It is easy to see that this is a generalization of the process of expanding a vector by writing out its projections on the Cartesian axes: $\vec{v} = v_1\vec{i} + v_1\vec{j} + v_3\vec{k}$.

Vector representation of functions

Because the representation of $f(x)$ as a series in $g_n(x)$ is unique, the function may be identified with the corresponding coefficients $\{a_1, a_2, a_3, \ldots\}$ that may be written out as elements of a column vector:

$$|f(x)\rangle = \sum_{n=1}^{\infty} a_n |g_n(x)\rangle \qquad \Leftrightarrow \qquad \vec{f} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

Such a vector is called a *representation* of the function $f(x)$ in the basis set $\{g_n(x)\}$. It will be demonstrated later in your quantum theory course that operators acting on functions can also undergo a similar procedure – they are represented with matrices.

Fourier series

One particular basis set is very important in practical applications. It is easy to demonstrate that the following set of complex exponentials (called *plane waves* in physics)

$$g_k(x) = e^{ikx}/\sqrt{2\pi} \qquad k = 0, \pm 1, \pm 2, \ldots$$

is orthonormal on the $x \in [-\pi, \pi]$ interval:

$$\langle g_n(x)|g_k(x)\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-inx}e^{ikx}dx = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(k-n)x}dx = \delta_{kn}$$

The corresponding series

$$f(x) = \sum_{-\infty}^{\infty} a_k e^{ikx} \qquad a_k = \langle e^{ikx}|f(x)\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi} f(x)e^{-ikx}dx$$

is called *Fourier series*. Expansions of this type form the foundation of digital signal processing, electromagnetism, quantum theory and theory of partial differential equations. Equivalent expressions may be given in terms of sines and cosines:

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

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)dx \qquad b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(nx)dx$$

Week 25 workshop exercises

1. Determine whether the following sets of functions are linearly independent (*i.e.* no function may be expressed as a linear combination of others):

   (a) $\{x, 1+x, 1-x\}$ (b) $\{\cos x, \cos 2x, \cos 3x\}$

   (c) $\{0, x\ln x, \arctan x, e^x\}$ (d) $\{\ln(x), \ln(x^2), \ln(x^3)\}$

2. Find the following norms and scalar products in the $x \in [-1,1]$ interval:

   (a) $\|x\|$ (b) $\|2^x\|$ (c) $\|\cos(\pi x/2)\|$

   (d) $\langle 1|x\rangle$ (e) $\langle x|2x^2-1\rangle$ (f) $\langle 2x^2-1|4x^3-3x\rangle$

3. Normalize the following functions on $x \in [-\pi, \pi]$ (find the value of N that would give a unit norm):

   (a) $f(x) = N$ (b) $f(x) = N\sin x$ (c) $f(x) = N^{-1}\cos(2x)$

   (d) $f(x) = N\sin^2 x$ (e) $f(x) = N(i - x/\pi)$ (f) $f(x) = Ne^{-4ix}$

4. Find the representation of the following functions in the plane wave basis set for $k = -1, 0, 1$:

   (a) $f(x) = \cos x$ (b) $f(x) = \sin x$ (c) $f(x) = 1$

Extra difficulty exercise for the brave

Atkins, "Molecular Quantum Mechanics", 5th edition: problems 1.2, 1.6, 1.7.

Find the Fourier series, up to (and including) the second harmonic for the following functions:

(a) $f(x) = x^2$ (b) $f(x) = x^3$ (c) $f(x) = |x|$

using *Mathematica* to take the difficult integrals. Compare each Fourier expansion to its original function by plotting both on the same graph.