1 Hilbert Space

1.1 Linear Algebra and Vector Spaces

The elements and operations of Hilbert space provides the machinery for quantum mechanics. Simply put, functions are viewed as vectors in a vector space. To begin with, examples of the inner product, completeness and orthonormality for vectors may be expressed in terms of R^3 co-ordinate space basis as:

$$(a,0,0)\cdot\begin{pmatrix}a\\0\\0\end{pmatrix}=a^2 \tag{1}$$

$$\begin{pmatrix}a\\b\\c\end{pmatrix}=a.\begin{pmatrix}1\\0\\0\end{pmatrix}+b.\begin{pmatrix}0\\1\\0\end{pmatrix}+c.\begin{pmatrix}0\\0\\1\end{pmatrix} \tag{2}$$

$$(0,1,0)\cdot\begin{pmatrix}0\\1\\0\end{pmatrix}=1;(1,0,0)\cdot\begin{pmatrix}0\\1\\0\end{pmatrix}=0 \tag{3}$$

In general, equation 1) is too exclusive, and a more flexible expression for complex vector spaces is:

$$(x,y)=\sum_{i=1}^{n}\xi_i^*\eta_i \tag{4}$$

which lends meaning to the idea of 'projection' of the 'dual' space vector x onto y ($x\neq y$) and 'length' or 'norm' ($x=y$), the latter written as $||x||$. A vector space which includes the inner product definition is referred to as an inner product space. By Schwarz's inequality, if x,y are vectors in this space, then

$$|(x,y)|\leq ||x||.||y|| \tag{5}$$

In 2), the basis is given implicitly and is said to 'span' R^3; an arbitrary vector in this space may always be expressed as a linear combination of these vectors. In 3) orthonormality is demonstrated using the basis. A set of vectors is orthonormal if each vector is orthogonal to every other in the set and normalized in unit length. Using an orthonormal set, a linear transformation can be represented as a matrix. More precisely, let V be an $n-$dimensional vector space, with $X=\{x_1,x_2,...,x_n\}$ a basis in V, and let A be a linear transformation mapping V into itself. Because any vector may be expressed as a linear combination of the basis, we have

$$Ax_j=\sum_{i=1}^{n}a_{ij}x_i \text{ for } j=1,...,n \tag{6}$$

The n^2 scalars a_{ij} constitute the matrix elements of linear transformation A relative to the basis X. With any square matrix such as A is associated a quantity referred to as the determinant, which may be defined as:

$$\det A=\sum_j A_{Jj}\ \mathrm{cof}(A_{Jj}) \tag{7}$$

for any row J. The cofactor (cof) of the element A_{Jj} is equal to $(-1)^{J+j}$ times the determinant of the $(n-1) \times (n-1)$ matrix obtained from A by eliminating the Jth row and jth column. This algorithm may be extended to columns:

$$\det A = \sum_j A_{jJ} \operatorname{cof} A_{jJ} \tag{8}$$

For example, if

$$A = a_{ij} = \begin{bmatrix} 1 & 3 & 5 \\ 4 & 3 & 2 \\ 1 & 3 & 2 \end{bmatrix} \tag{9}$$

the determinant is (along the first row):

$$\Delta = 1.(3.2 - 3.2) - 3.(4.2 - 2.1) + 5.(4.3 - 3.1) = 27 \tag{10}$$

or equivalently, by the second method (along the first column):

$$\Delta = 1.(3.2 - 3.2) - 4.(2.3 - 5.3) + 1.(2.3 - 3.5) = 27 \tag{11}$$

The determinant has a number of useful properties, including:

1. A common factor of each element of a row (or column) may be factored out as a multiplicative constant
2. An all zero row or column implies that det=0
3. det(AB)=det$A$.det$B$

The linear transformation A has an inverse with a matrix representation which depends on the determinant. For the previous example, the inverse is given by:

$$[A^{-1}]_{ij} = \frac{1}{\det A}[\text{adj}A]_{ij}$$

$$= \frac{1}{27}\begin{bmatrix} (-1)^{1+1}\det\begin{pmatrix} 3 & 2 \\ 3 & 2 \end{pmatrix} & (-1)^{2+1}\det\begin{pmatrix} 3 & 5 \\ 3 & 2 \end{pmatrix} & (-1)^{3+1}\det\begin{pmatrix} 3 & 5 \\ 3 & 2 \end{pmatrix} \\ (-1)^{1+2}\det\begin{pmatrix} 4 & 2 \\ 1 & 2 \end{pmatrix} & (-1)^{2+2}\det\begin{pmatrix} 1 & 5 \\ 1 & 2 \end{pmatrix} & (-1)^{3+2}\det\begin{pmatrix} 1 & 5 \\ 4 & 2 \end{pmatrix} \\ (-1)^{1+3}\det\begin{pmatrix} 4 & 3 \\ 1 & 3 \end{pmatrix} & (-1)^{2+3}\det\begin{pmatrix} 1 & 3 \\ 1 & 3 \end{pmatrix} & (-1)^{3+3}\det\begin{pmatrix} 1 & 3 \\ 4 & 3 \end{pmatrix} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & \frac{1}{3} & -\frac{1}{3} \\ -\frac{2}{9} & -\frac{1}{9} & \frac{2}{3} \\ \frac{1}{3} & 0 & -\frac{1}{3} \end{bmatrix} \tag{12}$$

where the adjoint (adj) matrix A_{ij} is equal to cof(A_{ji}). If the determinant is zero, then the matrix is said to be singular and no inverse exists. This may correspond physically to the case where the matrix elements are the coefficients in a set of linear equations which are not linearly independent. In this case there is insufficient information to determine to unknowns precisely.

Exercise: show that $AA^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I$

In general numerical methods are far more expedient in calculating the inverse. Also, one is at liberty to choose the basis which the elements of A are expressed with respect to. If in another basis the same transformation is C, then if there exists an invertible matrix B such that;

$$C = B^{-1}AB \tag{13}$$

then C is related to A by a similarity transformation. Similar matrices also share the same eigenvalues; a scalar λ is an eigenvalue and a nonzero vector x is an eigenvector of a linear transformation A if

$$Ax = \lambda x \tag{14}$$

Re-writing this as $(A - \lambda I)x = 0$, the only non-trivial solution for x dictates that $(A - I\lambda)$ be singular, ie.,

$$\det(A - \lambda I) = \det \begin{bmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} - \lambda & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} - \lambda \end{bmatrix} = 0 \tag{15}$$

For instance, if

$$A = \begin{bmatrix} 1 & -3 & 2 \\ -3 & 2 & 1 \\ 2 & 1 & 3 \end{bmatrix} \tag{16}$$

then by the previous procedure, this yields characteristic equation:

$$-\lambda^3 + 6\lambda^2 + 3\lambda - 42 = 0 \tag{17}$$

with solutions $\lambda = -2.4188, 3.6132, 4.8056$.
Exercise: The Hamilton-Cayley theorem states that a matrix obeys its own characteristic equation; show this for the previous example

One may write the corresponding eigenvectors as columns of a matrix P,

$$\begin{bmatrix} -0.725619 & -0.038605 & 0.687013 \\ -0.577350 & 0.577350 & -0.577350 \\ 0.374359 & 0.815583 & 0.441225 \end{bmatrix} \tag{18}$$

which is said to diagonalize A, since:

$$P^{-1}AP = \begin{bmatrix} -2.41883 & 0 & 0 \\ 0 & 3.61323 & 0 \\ 0 & 0 & 4.80560 \end{bmatrix} \tag{19}$$

In this example, all the eigenvalues (the 'spectrum') of the matrix A were real. While not stated explicitly, the matrix A given in the example is Hermitian. That is:

$$A = A\dagger \tag{20}$$

or in other words, a Hermitian matrix is one that is equal to the transpose (rows and columns are interchanged) of its complex conjugate (the two features of transposition and conjugation indicated by †). This ensures that the roots of the characteristic equation and hence eigenvalues are real. In quantum mechanics, the eignenvalues of an operator correspond to the result of a measurement. Therefore, observables must be Hermitian in nature. In addition, eigenvalues may have two types of multiplicity;

1. geometric multiplicity, meaning the number of linearly independent eigenvectors belonging to λ.
2. algebraic multiplicity, meaning the number of times λ appears as a root to the characteristic equation.

The physical implications in quantum mechanics are discussed in the appropriate section.

1.2 Sturm Liouville Systems

By analogy with the elements of linear algebra, one may produce similar definitions for functions, ie., the inner product:

$$(f_1, f_2) \equiv \int_a^b f_1^*(x) f_2(x) dx \tag{21}$$

completeness (Riesz-Fischer Theorem):

> Let the functions $f_1(x), f_2(x), ...$ be the elements in function space. If
>
> $$\lim_{n,m\to\infty} ||f_n - f_m||^2 \equiv \lim_{n,m\to\infty} \int_a^b |f_n(x) - f_m(x)|^2 dx = 0, \tag{22}$$
>
> there exists a square (Lebesgue) integral function $f(x)$ to which the sequence $f_n(x)$ converges 'in the mean'; ie., there exists an f such that:
>
> $$\lim_{n\to\infty} \int_a^b |f(x) - f_n(x)|^2 dx = 0 \tag{23}$$

and orthonormality:

$$(f_n, f_m) \equiv \int_a^b f_i^*(x) f_j(x) dx = \delta_{ij} \tag{24}$$

The implication is that an arbitrary (albeit continuous) function (by analogy to vectors) may be 'built up' as a linear combination of basis functions, these functions having the properties of completeness and orthonormality. This possibility is expressed in Weierstass's theorem for polynomials (eg., Hermite, Legendre etc), extended to trigonometric functions.

The functions (eg., Hermite, Legendre etc) of Hilbert Space may each be viewed as special solutions to a more general system. All the functions are solutions to an equation of the form

$$Lu = \lambda u \tag{25}$$

where

$$L = \alpha(x)\frac{d^2}{dx^2} + \beta(x)\frac{d}{dx} + \gamma(x) \tag{26}$$

λ is a constant and α, β, γ are real functions of x. The operators L are Hermitian:

$$(Lf, g) \equiv \int_{-\infty}^{\infty} (Lf(x))^* g(x) w(x) dx = \int_{-\infty}^{\infty} (f(x))^* (Lg(x)) w(x) dx \equiv (f, Lg) \tag{27}$$

(where $w(x)$ is a weight function) iff:

$$[w\alpha(f^* g' - g f^{*\prime})]_{-\infty}^{\infty} = 0$$

$$(w\alpha)' = w\beta \tag{28}$$

The last equation may be solved to give:

$$w\alpha = C \cdot \exp\left[\int \frac{\beta}{\alpha} dx\right] \tag{29}$$

Equation may be re-written as:

$$\frac{d}{dx}\left[w\alpha\frac{du}{dx}\right] + (\gamma - \lambda) w u \tag{30}$$

and with the condition (28) comprise a Sturm-Liouville (SL) system. One may show that eigenfunctions associated with distinct eigenvalues are orthogonal.
Exercise: Show this, ie., that:

$$(u_m, u_n) = \int_{-\infty}^{\infty} u_m^*(x) u_n(x) w(x) dx = 0 \tag{31}$$

The polynomial SL systems are special cases of the following polynomial coefficients:

$$\alpha(x) = \alpha_0 x^2 + \alpha_1 x + \alpha_2 \tag{32}$$

$$\beta(x) = \beta_0 x^2 + \beta_1 \tag{33}$$

$$\gamma(x) = \gamma_0 \tag{34}$$

Their properties are summarized in table 1.

Name	Differential Equation	$\alpha_0, \alpha_1, \alpha_2$	β_0	β_1	$w\alpha$	w	$[a,b]$
Jacobi	$(1-x^2)u'' + [-(p+q+2)x + (q-p)]u' + n(n+p+q+1)u = 0$	-1, 0, 1	$-(p+q+2)$	$q-p$	$(1-x)^{p+1}; (1+x)^{q+1}$	$(1-x)^p; (1+x)^q$	$[-1,1]$
Jacobi	$(x-x)u'' + [-(p+q+2)x + (p+1)]u' + n(n+p+q+1)$u=0	-1,1,0	$-(p+q+2)$	$p+1$	$x^{p+1}(1-x)^{q+1}$	$x^p(1-x)^q$	$[0,1]$
Gegenbauer	$(1-x^2)u'' - 2(m+1)xu' + n(n+2m+1)u = 0$	-1,0,1	$-2(m+1)$	0	$(1-x^2)^{m+1}$	$(1-x^2)^m$	$[-1,1]$
Tschebycheff	$(1-x^2)u'' - xu' + n^2u = 0$	-1,0,1	-1	0	$(1-x^2)^{1/2}$	$(1-x^2)^{-1/2}$	[-1,1]
Legendre	$(1-x^2)u'' - 2xu' + n(n+1)u = 0$	-1,0,1	-2	0	$1-x^2$	1	[-1,1]
Laguerre	$xu'' - [x-(s+1)]u' + nu = 0$	0,1,0	-1	$s+1$	$x^{s+1}e^{-x}$	$x^s e^{-x}$	$[0,\infty]$
Hermite	$u'' - 2xu' + 2nu$	0,0,1	-2	0	e^{-x^2}	e^{-x^2}	$[-\infty,\infty]$

Table 1: Sturm-Liouville systems