Infinite-Dimensional Linear Vector Spaces

The formal treatment of infinite-dimensional vector spaces is much more complicated than that of finite-dimensional vector spaces; in fact, the subject forms an entire branch of mathematics: *functional analysis*. These notes provide a non-rigorous overview, focusing on issues that will be important for quantum mechanics. One such is the requirement that the inner product $\langle W|V\rangle$ be finite, so that its modulus-squared can be interpreted as a probability (or probability density). Identification of the maximal set of vectors satisfying this requirement (i.e., ensuring the completeness of the vector space) can be a nontrivial matter.

Throughout what follows, "IPS" means "inner product space" (i.e., a linear vector space over the field of complex scalars that has an inner product).

The Dual Vector Space

- For any IPS $\mathbb{V}$, the *dual vector space* $\mathbb{V}^*$ is defined to be the set of bras $\langle W|$ that have a finite inner product $\langle W|V\rangle$ with every ket $|V\rangle$ in $\mathbb{V}$.
- For finite-dimensional IPS's, this definition implies that there is a 1:1 correspondence between the kets in $\mathbb{V}$ and the bras in $\mathbb{V}^*$. The correspondence is *antilinear*:
$$a|V\rangle + b|W\rangle \longleftrightarrow a^*\langle V| + b^*\langle W|.$$
- For infinite-dimensional IPS's, we shall see that $\mathbb{V}^*$ may be larger or smaller than $\mathbb{V}$.

IPS's With a Countably Infinite Basis

- Consider a countably infinite set of basis kets, denoted $\{|j\rangle, j = 1, 2, \ldots\}$, with a bra $\langle j|$ corresponding to each ket $|j\rangle$. Assume that the basis is orthonormal, i.e., $\langle j|k\rangle = \delta_{j,k}$. A generic ket can be written (uniquely) as $|V\rangle = \sum_{j=1}^{\infty} v_j|j\rangle$, where each v_j is a finite, complex number. There is a corresponding bra $\langle V| = \sum_{j=1}^{\infty} v_j^*\langle j|$. The inner product $\langle W|V\rangle = \sum_{j=1}^{\infty} w_j^* v_j$ can be represented as the contraction of an infinite row vector (the bra) with an infinite column vector (the ket).
- Many different infinite-dimensional IPS's can be composed from subsets of the set of all kets $|V\rangle$ defined above. We will consider three cases:

  1. An *incomplete IPS* $\mathbb{V}_0$ consisting of all finite linear combinations of the basis kets, i.e., all kets of the form $|V\rangle = \sum_{j=1}^{n} v_j|j\rangle$ where n is some positive integer. Each such ket can be represented as an infinite column vector with only a finite number of nonzero components. The dual vector space $\mathbb{V}_0^*$ consists of all bras having finite components in the basis $\{\langle j|\}$, irrespective of whether the number of nonzero components is finite or infinite. Therefore, $\mathbb{V}_0^*$ is much larger than $\mathbb{V}_0$.

     $\mathbb{V}_0$ is *incomplete* in the sense that there exist sequences of kets $|V_n\rangle$, $n = 1, 2, \ldots$, such that (i) $|V_n\rangle \in \mathbb{V}_0$ for all finite n; and (ii) the limit ket $|V_\infty\rangle = \lim_{n\to\infty}|V_n\rangle$ is well-defined and has a finite norm, but $|V_\infty\rangle \notin \mathbb{V}_0$. For instance, consider the sequence $|V_n\rangle = \sum_{j=1}^{n} j^{-1}|j\rangle$, for which $\langle V_\infty|V_\infty\rangle = \pi^2/6 < \infty$, but $|V_\infty\rangle$ lies outside $\mathbb{V}_0$ because it has an infinite number of nonzero components.

Example relevant to QM: The IPS $C[a,b]$ of all functions $f(x)$ that are continuous and square-integrable on a finite interval $[a,b]$, with the inner product defined as $\langle g|f\rangle = \int_a^b dx\, g^*(x)f(x)$. To see that this IPS is incomplete, consider the sequence of functions $f_n(x) = \arctan nx$, $n = 1, 2, \ldots$, defined on any finite interval that includes $x = 0$. Although $f_n(x) \in C[a,b]$ for all finite n, $\lim_{n\to\infty} f_n(x) = (\pi/2)\operatorname{sgn} x$ is discontinuous at $x = 0$, and therefore does not belong to $C[a,b]$.

2. A *Hilbert space* $\mathbb{V}_2$ consisting of all kets $|V\rangle$ having a finite norm $\sqrt{\sum_{j=1}^{\infty} |v_j|^2}$, irrespective of whether the number of nonzero components is finite or infinite. Formally, $\mathbb{V}_2$ is the *completion* of $\mathbb{V}_0$ with respect to the distance $||V - W||$: $\mathbb{V}_2$ contains all the vectors in $\mathbb{V}_0$, plus the limit of all convergent sequences $|V_n\rangle \in \mathbb{V}_0$, $n = 1, 2 \ldots$, with convergence being defined by $\lim_{n\to\infty} ||V_{n+1} - V_n|| = 0$. The correspondence between $\mathbb{V}_2$ and $\mathbb{V}_2^*$ is 1:1.

   Example relevant to QM: The IPS $L^2[a,b]$ of all complex-valued functions of one real argument that are square-integrable on the finite interval $[a,b]$: $L^2[a,b] = \{f(x) \mid \int_a^b dx|f(x)|^2 < \infty\}$. Fourier's theorem guarantees that this space has a countably infinite orthonormal basis $\{f_j(x)\}$ that is complete in the sense that any square-integrable $f(x)$ can be approximated to arbitrary accuracy via a Fourier sum: $\lim_{n\to\infty} ||f - \sum_{j=1}^{n} v_j f_j|| = 0$ for all $f \in L^2[a,b]$.

3. A *restricted IPS* $\mathbb{V}_R$ consisting of all kets $|V\rangle$ from $\mathbb{V}_2$ that satisfy some restriction stronger than having a finite norm. Since $\mathbb{V}_R$ is a subset of $\mathbb{V}_2$, every bra in $\mathbb{V}_2^*$ has a finite inner product with every ket in $\mathbb{V}_R$. In general, however, $\mathbb{V}_R^*$ is larger than $\mathbb{V}_2^*$, containing some bras from $\mathbb{V}^*$ that have a finite inner product with every ket in $\mathbb{V}_R$ but an infinite inner product with at least one ket from $\mathbb{V}_2$.

   Example: The set of all kets $|V\rangle$ from $\mathbb{V}_2$ that satisfy $\sum_{j=1}^{\infty} j^m |v_j|^2 < \infty$ for all positive integers m. (We'll see another example of a restricted IPS in the last section.)

Comparing these examples, we see that $\mathbb{V}_0 \subset \mathbb{V}_R \subset \mathbb{V}_2$ and $\mathbb{V}_2^* \subset \mathbb{V}_R^* \subset \mathbb{V}_0^*$, with only $\mathbb{V}_2 \longleftrightarrow \mathbb{V}_2^*$ being 1:1.

More on Hilbert Spaces

- A Hilbert space is any IPS that is complete with respect to the distance defined by the inner product. All finite-dimensional IPS's are complete, and hence they are Hilbert spaces, but this is not the case for all infinite-dimensional IPS's.

- In quantum mechanics, we deal only with *separable* Hilbert spaces: those that have a countable (finite or infinite) basis. The Hilbert space $L^2[a,b]$ defined above is separable.

- Another separable Hilbert space is the space $L^2 \equiv L^2[-\infty,\infty]$. It is not obvious that L^2 has a countably infinite basis because the natural generalization of the Fourier series to an infinite interval—the Fourier transform—involves a continuum of non-square-integrable basis functions of the form $\exp(ikx)$, $-\infty \le k \le \infty$. However, it turns out to be possible to reproduce any square-integrable $f(x)$ to arbitrary accuracy using a countable basis of orthonormal, square-integrable *wave packets*.

Coordinate and Plane-Wave Bases for $L^2[a,b]$ and L^2

- When working with the space $L^2[a,b]$ (on either a finite interval or the entire real line), it is useful to formally define the set $\{|x'\rangle,\ a \le x' \le b\}$, satisfying the orthonormality condition $\langle x'|x''\rangle = \delta(x'-x'')$. Here, $|x'\rangle$ represents a function that differs from zero only at $x = x'$, and $\langle x'|$ projects out the $x = x'$ component of an arbitrary ket $|f\rangle$, i.e., $\langle x'|f\rangle = f(x')$. The kets $|x'\rangle$ form a complete basis, in the sense that any ket in $L^2[a,b]$ can be written $|f\rangle = \int_a^b dx' f(x')|x'\rangle$. (Actually, the uncountable set $\{|x'\rangle\}$ forms an *overcomplete* basis, since $L^2[a,b]$ can be spanned using a countable basis.) The completeness relation for this basis is $\int_a^b dx'\,|x'\rangle\langle x'| = I$.

- Another useful basis for L^2 is the set $\{|k\rangle,\ -\infty \le k \le \infty\}$, satisfying the orthonormality condition $\langle k'|k''\rangle = \delta(k'-k'')$. Here $\langle x|k\rangle = \exp(ikx)/\sqrt{2\pi}$ is an infinite plane wave having wave vector k, and $\langle k|$ projects out the Fourier component of an arbitrary ket $|f\rangle$ at wave vector k, i.e., $\langle k|f\rangle = f(k) = \int_{-\infty}^{\infty} dx\, f(x)\exp(-ikx)/\sqrt{2\pi}$. The full ket can be written $|f\rangle = \int_{-\infty}^{\infty} dk\, f(k)|k\rangle$. (NB: For $L^2[a,b]$, one instead uses a countably infinite basis of unit-normalizable functions that are periodic on $[a,b]$.)

- The ket $|k\rangle$ defined above is an eigenket of the operator $K = -i\, d/dx$, which has the fundamental property that $K|f\rangle = |-i\, df/dx\rangle$ [hence, $\langle x'|K|f\rangle = -i\, df(x)/dx|_{x=x'}$]. The adjoint of this operator can be defined through its matrix elements:

$$\begin{aligned} \langle f|K^\dagger|g\rangle &= \langle g|K|f\rangle^* \\ \Rightarrow \quad \int_a^b dx\, f^*(x)K^\dagger g(x) &= \left(-i\int_a^b dx\, g^*(x)df(x)/dx\right)^* \\ &= \langle f|K|g\rangle + [if^*(x)g(x)]_a^b \qquad \text{(by parts).} \end{aligned}$$

  Therefore, the operator K is Hermitian (i.e., self-adjoint) only if the last term vanishes. This condition is satisfied if we consider only functions that vanish at $x = a$ and $x = b$, or if we restrict ourselves to functions that are periodic on the interval $a \le x \le b$. Less obviously (but see Shankar p. 66), the kets $|k\rangle$ can also be considered to meet the condition on the infinite line $[-\infty,\infty]$.

- Notice that $\langle x|x\rangle = \delta(0)$ "=" ∞, so $|x\rangle$ does not belong to $L^2[a,b]$ or L^2. (Strictly, $|x\rangle$ does not even represent a function, but rather a *distribution*.) Similarly, $\langle k|k\rangle = \delta(0)$ "=" ∞, so $|k\rangle$ does not belong to L^2. There are three ways to deal with this:

  1. Avoid using $\{|x\rangle\}$ and $\{|k\rangle\}$ at all. This solution is preferred by mathematical purists, but it is inconvenient for quantum mechanics because these kets turn out to be the eigenkets of the position and momentum operators, respectively.
  2. Describe physical states by kets $|\psi\rangle$ from a restricted IPS L_R of square-integrable functions that die off exponentially as $|x| \to \infty$, and eigenfunctions of operators by bras $\langle\omega|$ from the dual space L_R^*, which contains both $\{\langle x|\}$ and $\{\langle k|\}$. Calculate inner products $\langle\omega|\psi\rangle$, but never use $\{|\omega\}$. This solution is promoted by Ballentine.
  3. Work with a *physical Hilbert space* consisting of the Hilbert space of square-normalizable functions, augmented by all delta-function normalized functions. This is the practical solution adopted by the majority of physicists (without consciously thinking about it).