Introduction to Hilbert Spaces and their Applications in Quantum Mechanics

Pietro Faccioli

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Warning: these notes provide neither a complete nor a mathematically rigorous overview the theory of Hilbert Spaces. The purpose of these notes is, instead, merely that of giving a basic introduction to these concepts in the perspective of their applications to quantum mechanics. They are targeted for Master students in quantitative and computational biology.

1 From Vector to Hilbert Spaces

1.1 Basic Definitions

We recall that, in **classical mechanics**, the instantaneous state of a single particle is entirely specified by two vectors: the position $\mathbf{r}(t)$ and its momentum (or, equivalently, its velocity) $\mathbf{p}(t)$, which live in real vector spaces. The most important property of vector spaces is **linearity**: any linear combination of elements arbitrarily chosen inside the vector space $\mathcal{V}$ is still an element of the same vector space:

$$\text{For any } \mathbf{v}, \mathbf{w} \in V \text{ and } a, b \in R: \qquad a\mathbf{v} + b\mathbf{w} \in \mathcal{V} \tag{1}$$

Note that, here, we are specifically restricting to real vector spaces, i.e. requesting that $a, b \in R$. Vector spaces are usually equipped with an inner product (or, equivalently, scalar product), i.e. an operation taking as input two vectors and giving as output a scalar, specifically a real number for real vector spaces:

$$(\mathbf{v}, \mathbf{w}) \equiv \mathbf{v} \cdot \mathbf{w} = \mathbf{w} \cdot \mathbf{v} \in R. \tag{2}$$

The most important property of the scalar product is bi-linearity, i.e. linearity with respect to both vectors given in input:

$$(a_1\ \mathbf{v}_1 + a_2\ \mathbf{v}_2) \cdot (b_1\ \mathbf{w}_1 + b_2\ \mathbf{w}_1) = \sum_{i,k=1}^{2} a_i\ b_k\ \mathbf{v}_i \cdot \mathbf{w}_k. \tag{3}$$

In **quantum mechanics**, instead, the state of a particle is instantaneously described by a so-called quantum state $|\psi(t)\rangle$ that belongs to a new mathematical object called **Hilbert Space** – herby denoted with $\mathcal{H}$–. Hilbert spaces provide a suitable generalization of the notion of vector spaces, in a sense to be discussed below. The most important property of a Hilber Space is, therefore, that any linear combination of quantum states is still inside the Hilbert spaces:

$$\text{For any } |\psi\rangle, |\phi\rangle \in \mathcal{H} \text{ and } \alpha, \beta \in C: \qquad \alpha|\psi\rangle + \beta|\phi\rangle \in \mathcal{H} \tag{4}$$

Note that linear combinations are here defined with respect to complex coefficients (as opposed to real coefficients appearing in (1)). Just as in real vector spaces, in Hilbert spaces we can define a scalar product which takes as input to quantum states and gives as output a complex number:

$$\langle\psi|\phi\rangle = (\langle\phi|\psi\rangle)^* \in C. \tag{5}$$

Notice an important difference with respect the definition of inner product in a real vector space: in Hilbert spaces, reversing the order of elements in the inner spaces leads to the complex conjugate result. Just as in real vector spaces, the most important property of the inner product in $\mathcal{H}$ is its bi-liniearity:

$$\left\{ \begin{array}{l} |\xi\rangle \equiv \alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle \\ |\omega\rangle \equiv \beta_1|\phi_1\rangle + \beta_2|\phi_2\rangle \end{array} \right. \Rightarrow \langle\xi|\omega\rangle = \sum_{i=1}^{2} \alpha_i^* \beta_i \ \langle\psi_i|\phi_i\rangle$$

1.2 Complete orthonormal bases and projection

In standard vector spaces we are familiar with the concept of orthonormal basis vectors, i.e. a set form of elements which are mutually orthogonal and have unitary norm:

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \tag{6}$$

where δ_{ij} is the so-called Kronecker-Delta and is defined as follows:

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \tag{7}$$

(In passing note the following property of the Kronecker-Delta which will be used later:

$$\sum_j \delta_{ij} A_j = A_i \tag{8}$$

).

A set of N versors is said to form a *complete* orthonormal basis of the vector space $\mathcal{V}$ if for any vector $\mathbf{v} \in \mathcal{V}$ there exist a unique set of N real coefficients $\lambda_1, \ldots, \lambda_N$ which enable to express $\mathbf{v}$ as a linear combination of $\mathbf{e}_1, \ldots, \mathbf{e}_N$:

$$\mathbf{v} = \sum_{k=1}^{N} \lambda_k \ \mathbf{e}_k \tag{9}$$

In this case N is called the dimension of the vector space. The set of coefficients $\lambda_1, \ldots, \lambda_N$ are called the coordinates of the vector $\mathbf{v}$ in the given complete orthonormal basis $\{\mathbf{e}_k\}_{k=1,\ldots,N}$.

Similarly, a set of quantum states is defined to be a complete orthonormal basis of the Hilbert space $\mathcal{H}$ if (i) they are mutually orthogonal, (ii) have unit norm and (iii) if any state can be written as linear combination of them. However, a fundamental difference distinguishes bases of Hilbert spaces from bases of standard vector spaces: the elements of a complete orthonormal basis of a Hilbert space may form an infinite and dense set.

As practical example, let's consider the set of **position** quantum states $|\mathbf{x}\rangle$. Clearly, two positions can differ by an infinitesimal amount, therefore we need a continuous index $\mathbf{x}$ to label them. Two position states are said to obey the orthonormality condition if the following generalization of Eq. (6) holds

$$\langle \mathbf{x}|\mathbf{y}\rangle = \delta(\mathbf{x}-\mathbf{y}) \tag{10}$$

In this equation, however, $\delta(\mathbf{x}-\mathbf{y})$ denotes the so-called Dirac-delta, which is defined by a property which generalises Eq. (8) to summations over a continuous index (i.e. to integrals):

$$\int d^3\mathbf{y} A(y)\ \delta(\mathbf{x}-\mathbf{y}) = A(\mathbf{x}). \tag{11}$$

The fact that position states form a basis of $\mathcal{H}$ expresses the fact that any quantum state in the Hilbert space can obtained from a linear combination of the position states:

$$|\psi\rangle = \int d^3\mathbf{x}\ \phi(\mathbf{x})|\mathbf{x}\rangle \qquad \text{where} \quad \phi(\mathbf{x}) \in C \tag{12}$$

The complex function $\phi(\mathbf{x})$ is called the **wave function** and can be regarded as a dense and infinite set of complex coefficients (i.e. one for each different position $\mathbf{x}$). Therefore, Hilbert spaces are basically infinite dimension vector spaces.

1.3 Operators

In general operators are defined by their action on the elements of the vector space:

$$\mathbf{w} = \hat{O}\mathbf{v} \tag{13}$$

In particular, $\hat{O}$ is linear if

$$\hat{O}\left(\alpha_1\mathbf{v} + \alpha_2\mathbf{v_2}\right) = \alpha_1\hat{O}\mathbf{v_1} + \alpha_2\hat{O}\mathbf{v}_2 \tag{14}$$

Once a basis of a N-dimensional real vector space is defined, then each linear operator can be assigned a $N \times N$ matrix, through the following procedure (called "representation" of the operator in the specific basis):

$$\mathbf{w} = \hat{O}\mathbf{v} \Rightarrow w_j = \mathbf{e}_j \cdot \mathbf{w} = \sum_{i=1}^{N}(\mathbf{e}_i \cdot \mathbf{v})\mathbf{e_j} \cdot \hat{O}\mathbf{e}_i = \sum_{i=1}^{N} O_{ji}v_j \tag{15}$$

where $v_i = \mathbf{e}_i \cdot \mathbf{v}$ and $O_{ij} = \mathbf{e_i} \cdot \hat{O}\mathbf{e_j}$.

In complete analogy, a linear operator $\hat{O}$ defined in an Hilbert space $\mathcal{H}$ linearly maps a quantum state into another:

$$|w\rangle = \hat{O}|v\rangle \qquad \hat{O}\left(\alpha_1|v_1\rangle + \alpha_2|v_2\rangle\right) = \alpha_1\hat{O}|v_1\rangle + \alpha_2\hat{O}|v_2\rangle \tag{16}$$

Following exactly the same procedure outlined for real vector space, operators in Hilber spaces can be represented in a given orthonormal basis (e.g. the position state basis), through a projection procedure:

$$|\omega\rangle = \hat{O}|\psi\rangle \Rightarrow \omega(\mathbf{x}) = \langle \mathbf{x}|w\rangle = \int d^3\mathbf{y}\langle \mathbf{y}|\psi\rangle\langle \mathbf{x}|\hat{O}|\mathbf{y}\rangle = \int d^3\mathbf{y}\ O(\mathbf{x},\mathbf{y})\ \psi(\mathbf{y}) \quad (17)$$

where $\omega(\mathbf{x})$ and $\psi(\mathbf{x})$ denote the wave functions associated to the states $|\omega\rangle$ and $|\psi\rangle$, respectively. In most cases of interest, $O(\mathbf{x},\mathbf{y})$ is a nearly local operator. Here are some notable examples:

- Multiplicative operators: $U(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})u(y)$:

$$\int d^3\mathbf{y}\ U(\mathbf{x},\mathbf{y})\ \psi(\mathbf{y}) = u(\mathbf{x})\psi(\mathbf{x}) \qquad \text{(potential energy operator)} \quad (18)$$

- Derivative operators: $T(\mathbf{x},\mathbf{y}) = -\frac{\hbar^2}{2m}\delta(\mathbf{x}-\mathbf{y})\nabla^2_{\mathbf{x}}$:

$$\int d^3\mathbf{y}\ T(\mathbf{x},\mathbf{y})\ \psi(\mathbf{y}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) \qquad \text{(kinetic energy operator)} \quad (19)$$

2 Spectral Theorem

The spectral theorem is a fundamental result in the theory of linear operators in both vector and Hilbert spaces and specifies the general conditions under which operators can be diagolalized to yield a complete orthonormal basis.

Our starting point is to define the adjoint (or **Hermitian conjugate**) operator $O^\dagger$ of a generic linear operator $\hat{O}$, as one for which the following identity is satisfied (here expressed with the notation of vector spaces):

$$\langle \mathbf{v}\hat{O}^\dagger, \mathbf{w}\rangle = \langle \mathbf{v}, \hat{O}\mathbf{w}\rangle \quad (20)$$

An operator is called **Hermitian** if it is self-adjoint, i.e. of it coincides with its Hermitian conjugate: $\hat{O} = \hat{O}^\dagger$. Furthermore an operator $\hat{U}$ of is called **Unitary** if $\hat{U}^\dagger\hat{U} = 1$.

Spectral Theorem: Let $\hat{O}$ be an Hermitian operator defined on a Hilbert space $\mathcal{H}$. Then there exist a complete orthonormal basis of $\mathcal{H}$ defined by the eigenstates of $\hat{O}$. Furthermore, each eigenvalue is real.

Corollary 1: Hermitian matrices are such that $(O^T)^* = O$.

Corollary 2: Hermitian matrices in real vector space are symmetric.

Corollary 3: Given a complete orthonormal basis of a Hilbert space $\{|e_n\rangle\}$ (possibly dense) and a hermitian operator $\hat{O}$, it is possible to identify a unitary transformation which connects the $\{|e_n\rangle\}$ with the basis of eigenstates of $\hat{O}$, $\{|o_n\rangle\}$.

Note that the spectral theorem of standard linear algebra follows as a special case of this fundamental result.

3 Fourier Transform

A special case of basis change is provided by the so-called *Fourier transformation.* Let $\phi(\mathbf{x}$ be the wave function in coordinate representation. The unitary transformation to the momentum basis is called (direct) Fourier transform and is defined by:

$$\hat{F}[\phi(\mathbf{x})] = \tilde{\phi}(\mathbf{p}) = \int_{-\infty}^{\infty} d^3\mathbf{x}\ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}\ \phi(\mathbf{x}) \tag{21}$$

The inverse transformation (from the momentum basis to the position basis) is called the inverse Fourier transform:

$$\hat{F}^{-1}[\tilde{\phi}(\mathbf{p})] = \phi(\mathbf{x}) = \int_{-\infty}^{\infty} \frac{d^3\mathbf{p}}{(2\pi)^3}\ e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}\ \tilde{\phi}(\mathbf{p}) \tag{22}$$

Note that the $(2\pi)^{-3}$ in the inverse Fourier transform is conventionally introduced and guarantees the preservation of the normalization condition. In the mathematical literature sometimes authors adopt a slightly different convention, with factors $\sqrt{(2\pi)^3}$ appearing in denominators of both direct and inverse transforms.

An important property of Fourier transform is the following:

$$\begin{aligned} F^{-1}[\mathbf{p}\ \tilde{\phi}(\mathbf{p})] &= \int_{-\infty}^{\infty} \frac{d^3\mathbf{p}}{(2\pi)^3}\ e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}\ \mathbf{p}\ \tilde{\phi}(\mathbf{p}) \\ &= \left(-\frac{i\hbar}{\cancel{\hbar}}\frac{\partial}{\partial\mathbf{x}}\right)\int_{-\infty}^{\infty} \frac{d^3\mathbf{p}}{(2\pi)^3}\ e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}\tilde{\phi}(\mathbf{p}) \\ &= \left(-\frac{i\hbar}{\cancel{\hbar}}\frac{\partial}{\partial\mathbf{x}}\right)\phi(\mathbf{x}) \end{aligned} \tag{23}$$

where $\frac{\partial}{\partial\mathbf{x}}$ denotes the gradient operator.