Function Spaces

Application of linear algebra to function spaces

- vectors are (complex) functions of $x$,
- inner products are integrals,
- derivatives appear as linear transformations

Key points to understand:

- A class of functions behaves in a way similar to a set of vectors;
- An operator is similar to a linear transformation;
- A function space is a generalization of a linear space.
- This allows the use of linear algebra to the development of theory of quantum mechanics.
## Functions as Vectors

<table>
<thead>
<tr>
<th><strong>Vector</strong></th>
<th><strong>Function</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>The sum of two vectors is a vector;</td>
<td>The sum of two functions is a function.</td>
</tr>
<tr>
<td>Vector addition is commutative and associative;</td>
<td>Addition of functions is commutative and associative.</td>
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<tr>
<td>There exists a null vector such that $</td>
<td>\alpha\rangle +</td>
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<tr>
<td>The product of any scalar with any vector is another vector:</td>
<td>If we multiply a function by a complex number, we get another function.</td>
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<tr>
<td>A set of vectors, together with a set of scalars constitute a vector space.</td>
<td>Would the set of all functions constitute a vector space? We will be concerned with special <em>classes</em> of functions.</td>
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Inner Product

The inner product of two functions, \( f(x) \) and \( g(x) \), is defined by the integral

\[
\langle f | g \rangle = \int f(x)^* g(x) dx
\]

To have an inner product space, this integral must be well defined and finite. The necessary and sufficient condition for \( \langle f | g \rangle \) to be finite is that every admissible function be square integrable

\[
\int |f(x)|^2 dx < \infty
\]
Example: $P(N)$

Consider the set of all polynomials of degree $< N$.

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{N-1} x^{N-1}$$

on the interval $-1 \leq x \leq 1$. They are square integrable, so this is a inner product space. An obvious basis is

$$
|e_1\rangle = 1 \\
|e_2\rangle = x \\
|e_3\rangle = x^2 \\
\ldots \quad \ldots \quad \ldots \\
|e_N\rangle = x^{N-1}
$$

This is an $N$-dimensional vector space. However, it is not an orthonormal basis.

$$
\langle e_1 | e_1 \rangle = \int_{-1}^{1} 1 \, dx = 2, \quad \langle e_1 | e_3 \rangle = \int_{-1}^{1} x^2 \, dx = \frac{2}{3}
$$
Example: $P(N)$

The basis can be made orthonormal using the Gram-Schmidt procedure (to be discussed in tutorial). The results are the **Legendre polynomials**, $P_n(x)$.

\[ |e'_n\rangle = \sqrt{n - \frac{1}{2}} P_{n-1}(x), \quad (n = 1, 2, \ldots, n) \]

\[ |e'_1\rangle = \frac{1}{\sqrt{2}} P_0(x) = \frac{1}{\sqrt{2}} \]

\[ |e'_2\rangle = \sqrt{\frac{3}{2}} P_1(x) = \sqrt{\frac{3}{2}} x \]

\[ |e'_3\rangle = \sqrt{\frac{5}{2}} P_2(x) = \sqrt{\frac{5}{4}} (3x^2 - 1) \]

\[ \ldots \]

The new basis $|e'_n\rangle$ and the old basis $|e_n\rangle$ are related by a linear transformation.
Example

The wavefunctions of the one-dimensional harmonic oscillator form an inner product space. The wavefunctions

\[ \psi_n(x) = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2 / 2} \]

where

\[ \xi = \sqrt{\frac{m \omega}{\hbar}} x \]

can be used as basis. It is an orthonormal basis.

The wavefunctions of other systems, such as hydrogen atom, one-dimensional square well, etc. all have the same properties.
Operators as Linear Transformation

In function spaces operators (such as $d/dx$, $d^2/dx^2$, or simply $x$) behave as linear transformations, provided that they carry functions in the space into other functions in the space and satisfy the linearity condition:

$$\hat{T}(a|\alpha\rangle + b|\beta\rangle) = a(\hat{T}|\alpha\rangle) + b(\hat{T}|\beta\rangle)$$

For example, in the space of all polynomial of degree $< N$, $\hat{D} = d/dx$ is a linear transformation, but the operator $\hat{x}$ is not, for it takes $(N - 1)$th-order polynomial into $N$th-order polynomials, which are no longer in the space.

In a function space, the eigenvectors of an operator $\hat{T}$ are called \textbf{eigenfunctions}:

$$\hat{T}f(x) = \lambda f(x)$$
Example: $\hat{D}$

The eigenfunctions of the operator $\hat{D} = d/dx$ are

$$f_\lambda(x) = Ae^{\lambda x}$$

But $\hat{D}$ is not Hermitian!

For a Hermitian operator

$$\langle f | (\hat{T}|g) \rangle = (\langle f | \hat{T}^\dagger|g \rangle)$$

for all functions $f(x)$ and $g(x)$ in the space. Using integration by parts, we get

$$\langle f | (\hat{D}|g) \rangle = \int_a^b f^* \frac{dg}{dx} dx = (f^* g)|_a^b - \int_a^b \frac{df^*}{dx} g dx$$

$$= (f^* g)|_a^b - (\langle f | \hat{D}^\dagger|g \rangle).$$

An Hermitian operator can be constructed using $i\hat{D}$, and if we assume

$$f(b) = f(a)$$

The latter has no problem since in practice, we almost always work on the *infinite* interval ($a = -\infty$, $b = \infty$), and the square integrability guarantees that $f(\pm \infty) = 0$. 
Example: \( \hat{x} \)

Even though \( \hat{x} \) is not a linear transformation in the space of all polynomials of degree \(< N \) on the interval \(-1 \leq x \leq 1\), it can be a linear transformation in other spaces, such as the space of all polynomials (of degree \( \infty \)) on the interval \(-1 \leq x \leq 1\).

\( \hat{x} \) is Hermitian transformation!

\[
\int_{-1}^{1} [f(x)]^* [xg(x)] \, dx = \int_{-1}^{1} [xf(x)]^* [g(x)] \, dx.
\]

However, \( \hat{x} \) does not have any eigenfunctions in the space of all polynomials, because

\[ x(a_0 + a_1 x + a_2 x^2 + \cdots) \neq \lambda (a_0 + a_1 x + a_2 x^2 + \cdots) \]

The function satisfying the equation

\[ xg(x) = \lambda g(x) \]

is

\[ g_\lambda(x) = B \delta(x - \lambda) \]

i.e. the eigenfunctions of \( \hat{x} \) are Dirac delta functions.
Example: \( \hat{x} \)

This example illustrates that even though the first two theorems about Hermitian operator are completely general (the eigenvalues of a Hermitian operator are real, and the eigenvectors belonging to different eigenvalues are orthogonal), the third one (completeness of the eigenvectors) is valid (in general) only for finite-dimensional spaces.

In infinite-dimensional spaces some Hermitian operators have complete sets of eigenvectors, some have incomplete sets, and some have no eigenvectors (in the space) at all.

Unfortunately, the completeness property is absolutely essential in quantum mechanical applications.