Complex Variables and Vector Spaces

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Contents

Chapter 1

Vector Spaces

We wish to generalise the idea of a vector and field. Let us first define a field,

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Definition 1: Fields

A field $\mathbb{F}$ is a set with 2 binary operations defined on it, addition $(+)$ and multiplication $(\cdot)$. The following axioms hold $\forall a, b, c \in \mathbb{F}$,

1. *Associativity,*

$$a + (b + c) = (a + b) + c \qquad\qquad a \cdot (b \cdot c) = (a \cdot b) \cdot c \qquad (1.1)$$

2. *Commutativity,*

$$a + b = b + a \qquad\qquad a \cdot b = b \cdot a \qquad (1.2)$$

3. *Identity.* $\exists 0, 1 \in \mathbb{F}$ such that,

$$a + 0 = a \qquad\qquad a \cdot 1 = a \qquad (1.3)$$

4. *Additive inverse.* $\forall a \in \mathbb{F}, \exists -a \in \mathbb{F}$ such that,

$$a + (-a) = 0. \qquad (1.4)$$

5. *Multiplicative inverse.* $\forall a \in \mathbb{F}, \exists a^{-1} \in \mathbb{F}$ such that,

$$a \cdot a^{-1} = 1. \qquad (1.5)$$

We can then define a vector space,

Definition 2: Vector Space

Let $\mathbb{F}$ be a field. A vector space V over $\mathbb{F}$ is a set of objects $\mathbf{u}, \mathbf{v}, \mathbf{w}, \ldots$ which satisfy,

1. *Addition.* The set is closed under addition, such that $\mathbf{u}, \mathbf{v} \in V \implies \mathbf{w} = \mathbf{u} + \mathbf{v} \in V$. This operation is commutative and associative.

2. *Scalar multiplication.* The set is closed under multiplication by a scalar, i.e., $\mathbf{u} \in V \implies \lambda \mathbf{u} \in V$ for $\lambda \in \mathbb{F}$. Scalar multiplication is associative and distributive.

3. *Null vector.* $\exists \mathbf{0}, \mathbf{u} + \mathbf{0} = \mathbf{u}$.

4. *Negative vector.* $\forall \mathbf{u} \in V, \exists -\mathbf{u} \in V$ such that,

$$\mathbf{u} + (-\mathbf{u}) = 0. \qquad (1.6)$$

1.1   Linear Independence

If vectors are linearly independent, then they cannot be written as a combination of each other. Let us write down the formal definition,

> **Definition 3: Linear Independence**
>
> A set of vectors $\{\mathbf{u}_i \text{ for } i = 1, 2, \ldots, n\}$ is linearly independent if the equation,
>
> $$\sum_j^n \lambda_j \mathbf{u}_j = \mathbf{0} \tag{1.7}$$
>
> has only 1 solution, $\forall i : \lambda_i = 0$.

1.2   Postulate of Dimensionality and Basis Vectors

> **Definition 4: Dimensionality**
>
> A vector space V has dimensions N if it can accommodate no more than N linearly independent vectors $\mathbf{u}_j$.

We often denote N dimensional vector spaces over a field $\mathbb{F}$ as $\mathbb{F}^N$, or more generally V_N. We are often also interested in the *span* of a vector space.

> **Definition 5: Span**
>
> The span of a set of vectors $\{\mathbf{u}_i, for\, i = 1, 2, \ldots, n\}$ is the set of all vectors which can be written as a linear combination of $\mathbf{u}_i$.

The above definition naturally leads to the below theorem,

> **Theorem 1**
>
> In an N-dimensional vector space V_N, any vector $\mathbf{u}$ can be written as a linear combination of N linearly independent basis vectors $\mathbf{e}_j$.

Proof. Since there are no more than N linearly independent vectors, the set of vectors $\{\mathbf{e}_i\}_{i=1}^N + \mathbf{u}$ must be linearly dependent. Therefore, there must be a relation of the form,

$$\sum_{i=1}^N \lambda_i \mathbf{e}_i + \lambda_0 \mathbf{u} = \mathbf{0}, \tag{1.8}$$

where $\mathbf{u} \in V_N$ is an arbitrary vector and $\exists \lambda_i \neq 0$. From the definition of linear dependence, we require $\lambda_0 \mathbf{u}_0 \neq 0$, so,

$$\mathbf{u} = -\frac{1}{\lambda_0} \sum_{i=1}^N \lambda_i \mathbf{e}_i = \sum_i^N u_i \mathbf{e}_i \tag{1.9}$$

where $u_i = -\frac{\lambda_i}{\lambda_0}$. $\qquad\qquad\square$

From the above theorem, we are able to define the **basis** of a vector space,

> **Definition 6: Basis**
>
> Any set of N linearly independent vectors in V_n is called a **basis**, and then **span** V_N, or synonymously, they are **complete** if N is finite.

This allows us to write any vector $\mathbf{v} \in V_N$ as,

$$\mathbf{v} = \sum_i^N v_i \mathbf{e}_i \tag{1.10}$$

where $\mathbf{e}_i$ is any complete basis.

1.3 Linear Subspaces

We can consider a subspace of V_N as a vector space spanned by a set of $M < N$ linearly independent vectors. The subspace V_M must satisfy the following properties,

1. It must contain the zero vector $\mathbf{0}$.

2. It must be closed under addition and scalar multiplication.

An example of a subspace would be the subspace of $\mathbb{R}^3$ which is the set of vectors $(x, y, 0)$, where $x, y \in \mathbb{R}$ which define the xy-plane in $\mathbb{R}^3$. This is a case of a more general result,

> **Theorem 2: Subspaces**
>
> Any set of M $(M \leq N)$ linearly independent vectors $\{\mathbf{e}_i\}_{i=1}^M$ in V_N span a subspace V_M of V_N.

However, counterexamples do exist such as the set of vectors lying within a unit circle $\{(x, y) : x^2 + y^2 \leq 1\}$ which cannot be a subspace of $\mathbb{R}^3$ This is because we can choose a λ such that λx_1 or $\lambda y_1 > 1$ lies outside of the unit circle, and thus is not closed under multiplication.

1.4 Normed Spaces

We wish to now generalise length in order to define the closeness of vectors. We do this by defining a *norm*.

> **Definition 7: Norm**
>
> Give a vector space V over a field $\mathbb{F}$, a norm on V is a real-valued function $p : V \to \mathbb{R}$ with the following properties,
>
> 1. **Triangle Inequality**, $p(\mathbf{x} + \mathbf{y}) \leq p(\mathbf{x}) + p(\mathbf{y}), \forall \mathbf{x}, \mathbf{y} \in V$
>
> 2. **Absolute Homogeneity**, $p(sx) = |s|p(\mathbf{x}), \forall \mathbf{x} \in V, \forall s \in \mathbb{R}$.
>
> 3. **Positive Definiteness**, $\forall \mathbf{x} \in V, p(x) \geq 0; p(x) = 0 \iff x = 0$.

For a vector space V_N and two vectors $\mathbf{u}, \mathbf{v} \in V_N$, the distance between them is given by $\|\mathbf{u} - \mathbf{v}\|$. There are different types of norms, some of which are defined in sections below.

1.4.1 Supremum Norm

$\forall \mathbf{x} \in V_N$ where x_i are the components in a given basis, the we define the *supremum* or *infinity* norm.

> **Definition 8: Supremum Norm**
>
> $$\|\mathbf{x}\|_S = \|\mathbf{x}\|_\infty = \max_i |x_i|. \tag{1.11}$$

It can be shown that, since $|a + b| \leq |a| + |b| \ \forall a, b \in \mathbb{R}$ or $\forall a, b \in \mathbb{C}$,

$$\|\mathbf{x} + y\| = \max_i |x_i + y_i| \leq \max_i (|x_i| + |y_i|)$$
$$\leq \max_i |x_i| + \max_j |y| \tag{1.12}$$
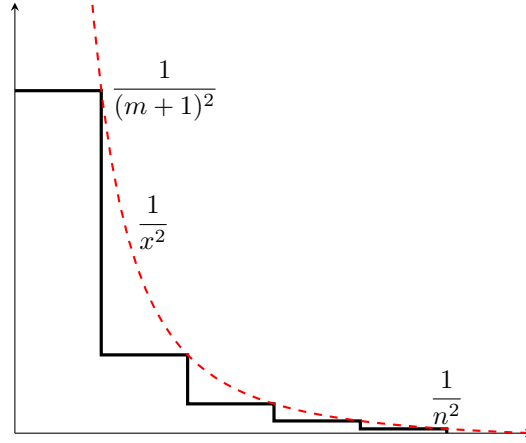
Figure 1.1: Graphical proof used in example 1.

1.4.2 1-Norm

$\forall \mathbf{x} \in V_N$ where x_i are the components of $\mathbf{x}$, we define the 1-norm,

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Definition 9: 1-Norm

$$\|x\|_1 = \sum_{i=1}^{N} |x_i|. \tag{1.13}$$

1.5 Completeness

1.5.1 Cauchy Sequences

Definition 10: Cauchy Sequence

A sequence $\{a_n\}_{n=0}^{\infty}$, $a_n \in V$ and V is a normed vector space is Cauchy if $\forall \epsilon > 0, \exists N > 0$ such that $\forall n, m > N, \|a_n - a_m\| < \epsilon$.

Let us consider some sequences and show if they are Cauchy.

Sequences over $\mathbb{R}$

Example 1: $a_n = \sum_{i=1} \frac{1}{i^2}$

A sequence in $\mathbb{R}$ with $\|a\| = |a|$ is

$$a_n = \sum_{i=1}^{n} \frac{1}{i^2}. \tag{1.14}$$

Is this sequence Cauchy?

For $n > m$, let us write,

$$|a_n - a_m| = \sum_{i=m+1}^{n} \frac{1}{i^2} \tag{1.15}$$

If we consider the sum as the integral over a series of step functions, then we can consider an approxi-

mation of this integral as $\frac{1}{x^2}$, as in figure 1.1. Thus,

$$\sum_{i=m+1}^{n} \frac{1}{i^2} \leq \int_{m}^{n} \frac{1}{x^2} \, dx$$

$$= \frac{1}{n} - \frac{1}{m} \leq \frac{1}{n} \leq \frac{1}{N}. \tag{1.16}$$

Let us now choose $N > \frac{1}{\epsilon}$, so that we find,

$$|a_n - a_m| < \epsilon \tag{1.17}$$

thus the sequence is Cauchy. □

> **Example 2:** $a_n = n$
>
> onsider a sequence $a_n = n$. Is this sequence Cauchy?

Let us choose $\epsilon = 1$, $n = N + 1$, and $m = N + 3$

$$|a_n - a_m| = 2 > \epsilon \tag{1.18}$$

so the sequence is not Cauchy. □

Cauchy sequences of functions

We can also apply similar proofs to functions.

> **Example 3:** $f : [0, 1] \rightarrow \mathbb{R}$, $f_n(x) = \frac{x}{n}$.
>
> Consider $f : [0, 1] \rightarrow \mathbb{R}$ where $f_n(x) = \frac{x}{n}$. Is this function Cauchy?

Let $n > m$,

$$\|f_n - f_m\|_1 = \int_0^1 \left| \frac{x}{n} - \frac{x}{m} \right| dx$$

$$= \left| \frac{1}{n} - \frac{1}{m} \right| \int_0^1 x \, dx \tag{1.19}$$

$$= \frac{1}{2} \left| \frac{1}{n} - \frac{1}{m} \right| \leq \frac{1}{2} \left(\left| \frac{1}{n} \right| + \left| \frac{1}{m} \right| \right) \leq \frac{1}{2} \frac{2}{N} = \frac{1}{N}.$$

Choose $N > 1/\epsilon \implies \|f_n - f_m\| < \epsilon$, so f is Cauchy.

1.5.2 Cauchy Sequences and Convergence

Every convergent sequence is Cauchy, because if $a_n \rightarrow x \implies \|a_m - a_n\| \leq \|a_m - x\| + \|x - a_n\|$ both of which go to zero. Whether every Cauchy sequence is convergent gives rise to the following definition,

> **Definition 11: Completeness**
>
> A field is complete if every Cauchy sequence in the field converges to an element of the field.

> **Example 4: Completeness of $\mathbb{Q}$**
>
> Consider $a_n = \frac{a_{n-1}}{2} + \frac{1}{a_{n-1}}$. Let us assume a_∞ exists.
>
> $$a_\infty = \frac{a_\infty}{2} + \frac{1}{a_\infty} \tag{1.20}$$
>
> $\implies \frac{1}{2} a_\infty^2 = 1 \implies a_\infty = \sqrt{2} \notin \mathbb{Q} \therefore \mathbb{Q}$ is not complete. □
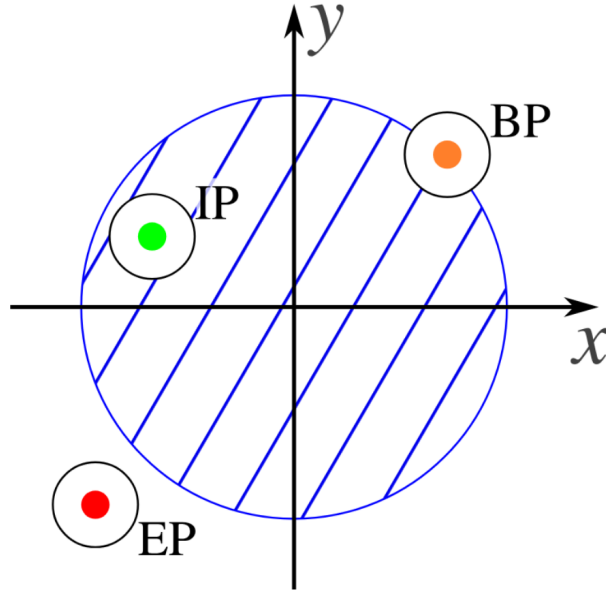
Figure 1.2: Interior point (IP), exterior point (EP), and boundary point (BP).

1.6 Open and Closed Sets

Now that we have defined completeness, let us look at the difference between open and closed sets, particularly on the 2D plane. We will be considering a ball in the 2D plane, defined,

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Definition 12: Ball

A ball of radius ϵ around a point $\mathbf{r}_0$ is the set of all points $\mathbf{r}$ such that $\|\mathbf{r} - \mathbf{r}_0\|$.

A sphere is the points where $\|\mathbf{r} - \mathbf{r}_0\| = \epsilon$. Let us denote the set of the sphere S. We will consider three types of points, visualised in figure 1.2,

- **Exterior point**, for some ϵ, all $\mathbf{r} \notin S$.

- **Interior point**, for some ϵ, all $\mathbf{r} \in S$.

- **Boundary point**, for some ϵ, some of the neighbourhood of $\mathbf{r} \in S$ and some $\mathbf{r} \notin S$.

We can then define closed and open sets.

Definition 13: Closed Set

A set that contains all its boundary points is closed.

An example of this is a set of points $|r| \leq 1$, as $|r| = 1$ is a boundary point, and also belongs to the set.

Definition 14: Open Set

A set that only includes interior points is open.

We must furthmore define,

Definition 15: Connected Set

Sets for which any two points can be joined by a continuous path.

If a set is connected and open, we call it a *region*.

> **Example 5**
>
> The function $f(z) = \frac{1}{(1-z)}$ has a defined Taylor series for $z \neq 1$,
>
> $$f(z) = \sum_{i=0}^{\infty} z^i. \tag{1.21}$$
>
> For what complex numbers is this series Cauchy? Is this an open or closed set?

We will consider the cases $|z| < 1$ and $|z| > 1$ separately, with $|z| = 1$ as a boundary case. Let us define,

$$a_n = \sum_{i=0}^{n} z^i. \tag{1.22}$$

For any $z \neq 1$, assuming $n > m$,

$$|a_n - a_m| = \left| \sum_{i=m+1}^{n} z_i \right| = \left| \frac{z^{m+1} - z^{n+1}}{1-z} \right|. \tag{1.23}$$

For $|z| < 1$,

$$|a_n - a_m| = \frac{|z|^m}{|1-z|} \left| 1 - z^{n-m+1} \right| \leq \frac{2}{|1-z|} |z|^m \tag{1.24}$$

and since $|z|^m$ is decreasing as a function of m, the series is Cauchy. For $|z| > 1$,

$$|a_n - a_m| = \frac{|z|^n}{|1-z|} \left| 1 - z^{-n+m+1} \right| \geq \frac{2}{|1 - \frac{1}{z}|} |z|^n = z^{n+1} \tag{1.25}$$

and since $|z|^n$ is an increasing function of n, the series is not Cauchy. Thus the series is Cauchy in the open set $|z| < 1$.

1.7 Inner Product Space

An inner product space is a vector space with an inner product, which is a generalisation of the scalar product.

> **Definition 16: Inner product, $\langle \mathbf{a}, \mathbf{b} \rangle$**
>
> Given a vector space V_N over $\mathbb{F}$, the inner product between two vectors $\mathbf{a}, \mathbf{b} \in V_N$ is a function such that $V \times V \to \mathbb{F}$. If $\mathbb{F} \subset \mathbb{C}$, the following properties hold,
>
> 1. **Linearity.** If $\mathbf{w} = \lambda \mathbf{u} + \mu \mathbf{v}$ then $\langle \mathbf{a}, \mathbf{w} \rangle = \lambda \langle \mathbf{a}, \mathbf{u} \rangle + \mu \langle \mathbf{a}, \mathbf{u} \rangle$.
> 2. **Conjugation Symmetry.** $\overline{\langle \mathbf{w}, \mathbf{a} \rangle} = \langle \mathbf{a}, \mathbf{w} \rangle$
> 3. **Positive Definiteness.** $\forall \mathbf{x} \neq 0, \langle \mathbf{x}, \mathbf{x} \rangle > 0$.

From our definition of the inner product, we can define the 2-norm,

$$\|\mathbf{a}\|^2 = \langle \mathbf{a}, \mathbf{a} \rangle \geq 0. \tag{1.26}$$

1.7.1 Orthogonality

> **Definition 17: Orthogonality**
>
> $\forall \mathbf{a}, \mathbf{b} \neq 0 \in V_N$ if $\langle \mathbf{a}, \mathbf{b} \rangle = 0$ then $\mathbf{a}$ and $\mathbf{b}$ are orthogonal.

This allows us to then define an orthonormal basis.

Definition 18: Orthonormal basis

The set basis vectors $\{\mathbf{e}_i\}_{i=1}^N \in V_N$ is orthogonal if,

$$\langle \mathbf{e}_i, \mathbf{e}_j \rangle = A_i \delta_{ij}. \tag{1.27}$$

and $A_i \neq 0$. The set of basis vectors is orthonormal for $A_i = 1, \forall i \in [1, N]$.

Given we can decompose any vector $\mathbf{a} \in V_N$ if given a complete set of basis vectors, we can define a general inner product for V_N over $\mathbb{F} \subset \mathbb{C}$. Let us begin by writing the decomposition of two vectors $\mathbf{a}, \mathbf{b} \in V_N$ into a set of basis vectors $\{\mathbf{e}_j\}_{j=1}^N$,

$$\mathbf{a} = \sum_{j=1}^N a_j \mathbf{e}_j \qquad\qquad \mathbf{b} = \sum_{j=1}^N b_j \mathbf{e}_j. \tag{1.28}$$

Then, using linearity,

$$\begin{aligned}
\langle \mathbf{a}, \mathbf{b} \rangle &= \sum_{j,k=1}^N \overline{a}_j \langle \mathbf{e}_j, \mathbf{e}_k \rangle b_k \\
&= \sum_{i,j=1}^N \overline{a}_j \delta_{jk} b_k \\
&= \sum_{j=1}^N \overline{a}_j b_j.
\end{aligned} \tag{1.29}$$

NOTE: This only holds when using an orthonormal basis.

We can obtain further insight into the decomposition of a vector by considering the inner product,

$$\mathbf{a} = \sum_{j=1}^N a_j \mathbf{e}_j \implies \langle \mathbf{e}_k, \mathbf{a} \rangle = \sum_{j=1}^N a_j \underbrace{\langle \mathbf{e}_j, \mathbf{e}_k \rangle}_{\delta_{jk}} = a_k. \tag{1.30}$$

We often refer to $a_k = \langle \mathbf{e}_k, \mathbf{a} \rangle$ as the *projection* of $\mathbf{a}$ onto $\mathbf{e}_k$ as it gives the component of $\mathbf{a}$ in the $\mathbf{e}_k$ direction.

1.7.2   Gram-Schmidt Orthonormalisation

Definition 19: Gram-Schmidt Algorithm

Given a basis $\{\mathbf{v}_j\}_{j=1}^N \in V_N$,

1. Define
$$\mathbf{e}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|} \tag{1.31}$$

2. Define
$$\mathbf{u}_2 = \mathbf{v}_2 - \langle \mathbf{e}_1, \mathbf{e}_2 \rangle \mathbf{e_1} \qquad\qquad \mathbf{e}_2 = \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \tag{1.32}$$

$\vdots$

m. Define,
$$\mathbf{u}_m = \mathbf{v}_m - \sum_{j=1}^{m-1} \langle \mathbf{e}_j, \mathbf{v}_m \rangle \mathbf{e}_j \tag{1.33}$$

thus,
$$\mathbf{e}_m = \frac{\mathbf{u}_m}{\|\mathbf{u}_m\|} \tag{1.34}$$

> up to N.

The Gram-Schmidt process is able to take any set of basis vectors and turn it into a set of orthonormal basis vectors. The idea behind it is that given 2 vectors $\mathbf{v}, \mathbf{u}$ such that $\|\mathbf{u}\| = 1$, then we wish to define a vector $\mathbf{v}' = \mathbf{v} - \langle \mathbf{u}, \mathbf{v} \rangle \mathbf{u}$. The inner product with $\mathbf{u}$ and this new vector is then,

$$\langle \mathbf{u}, \mathbf{v}' \rangle = \langle \mathbf{u}, \mathbf{v} \rangle - \langle \mathbf{u}, \mathbf{v} \rangle \overset{1}{\cancel{\langle \mathbf{u}, \mathbf{u} \rangle}} = 0. \tag{1.35}$$

So, we essentially are removing the non-orthonormal components from each subsequent basis vector, based on the first basis vector in the set.

1.7.3 Inequalities of Inner Product Space

Theorem 3: Cauchy-Schwartz Inequality

$\forall \mathbf{a}, \mathbf{b} \in V_N, |\langle \mathbf{a}, \mathbf{b} \rangle| \leq \|\mathbf{a}\| \|\mathbf{b}\|.$

Proof. Consider $\mathbf{u} = \mathbf{a} - \lambda \mathbf{b}$,

$$\|\mathbf{a}\|^2 = \|\mathbf{a}\|^2 + |\lambda|^2 \|\mathbf{b}\|^2 - \overline{\lambda} \langle \mathbf{b}, \mathbf{a} \rangle - \lambda \langle \mathbf{a}, \mathbf{b} \rangle \geq 0. \tag{1.36}$$

Choose,

$$\lambda = \frac{\langle \mathbf{b}, \mathbf{a} \rangle}{\|\mathbf{b}\|^2}. \tag{1.37}$$

Thus,

$$\|\mathbf{u}\|^2 = \|\mathbf{a}\|^2 \|\mathbf{b}\|^2 - \frac{|\langle \mathbf{a}, \mathbf{b} \rangle|}{\|\mathbf{b}\|^2} \geq 0 \tag{1.38}$$

$\implies |\langle \mathbf{a}, \mathbf{b} \rangle| \leq \|\mathbf{a}\| \|\mathbf{b}\|.$ □

Theorem 4: Triangle Inequality

$\forall \mathbf{a}, \mathbf{b} \in V_N, \|\mathbf{a} + \mathbf{b}\| \leq \|\mathbf{a}\| + \|\mathbf{b}\|$

Proof.

$$\begin{aligned}
\|\mathbf{a} + \mathbf{b}\|^2 &= \langle \mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{b} \rangle \\
&\leq \|\mathbf{a}\|^2 + \|\mathbf{b}\|^2 + 2|\langle \mathbf{a}, \mathbf{b} \rangle| \\
&\leq \|\mathbf{a}\|^2 + \|\mathbf{b}\|^2 + 2\|\mathbf{a}\| \|\mathbf{b}\| = (\|\mathbf{a}\| + \|\mathbf{b}\|)^2
\end{aligned} \tag{1.39}$$

$\implies \|\mathbf{a} + \mathbf{b}\| \leq \|\mathbf{a}\| + \|\mathbf{b}\|$ □

1.8 Function Space

We denote function spaces by $\mathcal{F}$. Let us define the function space inner product.

Definition 20: Function Space Inner Product

For $x \in [a, b]$, and functions $f, g : [a, b] \to \mathbb{C}$, the inner product is given by

$$\langle f | g \rangle = \int_a^b \overline{f(x)} g(x) \mathrm{d}\mu(x) \tag{1.40}$$

where $\mathrm{d}\mu(x)$ is the integration measure of a function space.

The inner product must satisfy,

$$\|f\|^2 = \langle f|f \rangle = \int_a^b |f(x)|^2 \mathrm{d}\mu(x) \geq 0 \tag{1.41}$$

which is only 0 if $f(x) = 0 \forall x$. If $\|f\|^2$ is finite, then f is square-integrable and can be normalised. Function spaces where all functions are square-integrable are known as Hilbert spaces.

Definition 21: L2 Functions

A function f is said to be in the space $L^2([a,b])$ if $\|f\|^2 = \int_a^b |f(x)|^2 \mathrm{d}\mu(x) < \infty$.

Let us note that we will use $\mathrm{d}\mu(x) = \mathrm{d}x$ throughout the course, however most concepts can be generalised to an arbitrary measure.

1.8.1 Basis functions and completeness

A function $f \in \mathcal{F}$ over the domain $x \in [a,b]$ can be represented by a set of basis vectors $\{u_n\}_{n=1}^\infty \in \mathcal{F}$ as,

$$f(x) = \sum_{n=1}^\infty f_n u_n(x) \tag{1.42}$$

where the coefficients f_n are defined,

$$f_n = \langle u_n|f \rangle = \int_a^b \overline{u_n(x)} f(x) \, \mathrm{d}x \,. \tag{1.43}$$

We can define the completeness relation for an infinite function space by,

$$\sum_{n=1}^\infty u_n(x) \overline{u_n(y)} = \delta(x-y). \tag{1.44}$$

1.8.2 Coordinate Representation

When we write $f(x)$, we are referring to a function $f \in \mathcal{F}$ in a basis defined by the coordinate x. Let us write this more explicitly, calling $|x\rangle$ the *position vector*, and writing $f \in \mathcal{F}$,

$$|f\rangle = \int_a^b \mathrm{d}x \, f(x) \, |x\rangle \tag{1.45}$$

where we integrate rather than sum since position is continuous. We can then clearly see,

$$f(x) = \langle x|f \rangle = \int_a^b \delta(y-x) f(y) \, \mathrm{d}y \tag{1.46}$$

from which we find that the Dirac-delta acts as a basis vector for position vectors. We define the overlap of two position vectors,

$$\langle x|x' \rangle = \int_a^b \delta(y-x)\delta(y-x') \, \mathrm{d}y = \delta(x-x') \iff x, x' \in [a,b] \,. \tag{1.47}$$

The completeness relation is then,

$$\int_a^b |x\rangle \langle x| \, \mathrm{d}x = \hat{\mathbb{1}}. \tag{1.48}$$

Chapter 2

Linear Operators

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Definition 22: Map

A map M is a function which takes $V \to W$ where V, W are vector spaces. This is such that M acting on $\mathbf{c} \in V$ produces a different vector $\mathbf{c}' \in W$.

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We are often interested in linear maps, or linear operators as they are often called in physics.

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Definition 23: Linear Operator

An operator $\hat{A}$ is linear if, for a vector $\mathbf{c} = \lambda \mathbf{a} + \mu \mathbf{b}$ where $\forall \lambda, \mu \in \mathbb{F}$ and $\forall \mathbf{a}, \mathbf{b} \in V$ over $\mathbb{F}$,

$$\mathbf{c}' = \hat{A}\mathbf{c} = \mu(\hat{A}\mathbf{a}) + \lambda(\hat{A}\mathbf{b}) \tag{2.1}$$

</div>

In physics, but not generally, linear operators always map $V \to V$.

2.1 Algebra of operators

We can define the following properties of linear operators,

1. $(\hat{A} + \hat{B}) \equiv \hat{A}\mathbf{v} + \hat{B}\mathbf{v}$.

2. $(\lambda \hat{A})\mathbf{v} = \lambda(\hat{A}\mathbf{v})$.

3. $\exists \hat{\mathbb{1}} : \hat{\mathbb{1}}\mathbf{v} = \mathbf{v}, \forall \mathbf{v} \in V$.

4. $\exists \hat{0} : \hat{0}\mathbf{v} = \mathbf{0}, \forall \mathbf{v} \in V$.

5. $\forall \mathbf{v} \in V, (\hat{B}\hat{A})\mathbf{v} = \hat{B}(\hat{A}\mathbf{v})$, generally $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

2.2 Matrix Representation of Linear Operators

Consider V_N over $\mathbb{F}$. Assume $\{\mathbf{e}_j\}_{j=1}^N$ is an orthonormal basis. $\forall \mathbf{v} \in V_N$,

$$\mathbf{v} = \sum_{j=1}^N v_j \mathbf{e}_j \tag{2.2}$$

where $\langle \mathbf{e}_k, \mathbf{v} \rangle = v_k$. Given a linear operator $\hat{A}$,

$$\hat{A}\mathbf{v} = \hat{A}\left(\sum_{j=1}^N v_j \mathbf{e}_j\right) = \sum_{j=1}^N v_j \hat{A}\mathbf{e}_j \tag{2.3}$$

by linearity. We have $\hat{A}\mathbf{e}_j \in V_N$, thus,

$$\hat{A}\mathbf{e}_j = \sum_{i=1}^{N} \mathbf{e}_i \underbrace{(\hat{A}\mathbf{e}_j)}_{A_{ij}} \tag{2.4}$$

so,

$$\hat{A}\mathbf{e}_j = \sum_{i=1}^{N} \mathbf{e} A_{ij}$$
$$\implies A_{ij} = \langle \mathbf{e}_i, \hat{A}\mathbf{e}_j \rangle. \tag{2.5}$$

So,

$$\hat{A}\mathbf{v} = \sum_{j=1}^{N} v_j \sum_{i=1}^{N} (A_i j \mathbf{e}_i)$$
$$= \sum_{i=1}^{N} \left(\sum_{j=1}^{N} A_{ij} v_j \right) \mathbf{e}_i \tag{2.6}$$

thus,

$$(\hat{A}\mathbf{v})_i = \sum_{j=1}^{N} A_{ij} v_j. \tag{2.7}$$

Interestingly, we have obtained matrix multiplication from linearity and orthonormality, rather than having to define it.

2.3   Inverse Operator

> **Definition 24: Inverse operator**
>
> Given an operator $\hat{A}$ from $V \to V$, $\forall \mathbf{v} \in V$, $\exists \hat{B}$ such that, $\hat{B}(\hat{A}\mathbf{v}) = \mathbf{v}$, $(\hat{B}\hat{A})\mathbf{v} = \mathbf{v} \implies \hat{B}\hat{A} = \hat{\mathbb{1}}$. We call $\hat{B} = \hat{A}^{-1}$.

NOTE: Not all operators have an inverse.

2.4   Dyadic (Outer) Product

Recall $\langle u | \hat{A} | v \rangle \to \mathbf{u}^\dagger \hat{A}\mathbf{v}$, or $\langle \mathbf{u}, \hat{A}\mathbf{v} \rangle$. We can clearly see that $\mathbf{c}\langle \mathbf{a}, \mathbf{b} \rangle$ is a vector. Let us define,

$$\mathbf{c}' = \mathbf{c}(\mathbf{a}^\dagger \mathbf{b}) = \underbrace{(\mathbf{ca}^\dagger)}_{\substack{\text{Linear} \\ \text{Operator}}} \mathbf{b} \tag{2.8}$$

this linear operator is known as a *dyad* or the *outer product* of $\mathbf{a}$ and $\mathbf{c}$. Let us define it more formall,y

> **Definition 25: Dyad/Outer product**
>
> For $V_N \subset \mathbb{C}^N$, and vectors $\mathbf{a}, \mathbf{b} \in V_N$, their outer product is defined $\mathbf{ab}^\dagger$. It has the following properties,
>
> 1. **Linearity in the first argument**. If $\mathbf{c} = \lambda\mathbf{a} + \mu\mathbf{b}$, then $\mathbf{cd}^\dagger = \lambda\mathbf{ad}^\dagger + \mu\mathbf{bd}^\dagger$.
>
> 2. **Antilinearity in the second argument**. If $\mathbf{d} = \lambda\mathbf{a} + \mu\mathbf{b}$, then $\mathbf{cd}^\dagger = \bar{\lambda}\mathbf{ca}^\dagger + \bar{\mu}\mathbf{cb}^\dagger$.

2.5   Projection Operator and the Completeness Relation

If $\hat{P}^2\mathbf{v} = \hat{P}\mathbf{v}$, $\forall \mathbf{v} \in V_N$, then $\hat{P}$ is a projection operator. For a given orthonormal basis $\{\mathbf{e}_j\}_{j=1}^{N} \in V_N$, $\hat{P}_j = \mathbf{e}_j\mathbf{e}_j^{\dagger}$. A consequence of this is the completeness relation,

$$\sum_{j=1}^{N} \hat{P}_j = \sum_{j=1}^{N} \mathbf{e}_j\mathbf{e}_j^{\dagger} = \hat{\mathbb{1}}. \tag{2.9}$$

2.6   The Adjoint or Hermitian Conjugate

Definition 26: Adjoint

$$\forall \hat{A}, \forall \mathbf{u}, \mathbf{v} \in V_N : \langle \mathbf{u}, \hat{A}^{\dagger}\mathbf{v} \rangle = \overline{\langle \mathbf{v}, \hat{A}\mathbf{u} \rangle} \tag{2.10}$$

In matrix notation,

$$(\hat{A}^{\dagger})_{ij} = \overline{A_{ji}}. \tag{2.11}$$

An operator is self adjoint if $\hat{A} = \hat{A}^{\dagger}$.

Definition 27: Unitary Operator

$$\exists \hat{U} : \hat{U}^{\dagger}\hat{U} = \hat{U}\hat{U}^{\dagger} = \hat{\mathbb{1}} \tag{2.12}$$

i.e.,

$$\hat{U}^{-1} = \hat{U}^{\dagger}. \tag{2.13}$$

2.7   Representations

2.7.1   Representation of a Vector

We know that a vector can be decomposed into orthonormal basis vectors. A vector space can have more than one set of orthonormal basis vectors which can represent a given vector. From the completeness relation, we find,

$$\begin{aligned} \mathbf{v} = \hat{\mathbb{1}}\mathbf{v} &= \sum_{j=1}^{N} \langle \mathbf{e}_j, \mathbf{v} \rangle \mathbf{e}_j \\ &= \sum_{j=1}^{N} \langle \mathbf{f}_j, \mathbf{v} \rangle \mathbf{f}_j \end{aligned} \tag{2.14}$$

i.e., changing basis does not change the abstract concept of a vector.

Invariance of the Inner Product

We can emphasise the idea above by considering the inner product of a vector. We can write some vector $\mathbf{v} \in V_N$ as,

$$\mathbf{v} = \sum_{j=1}^{N} a_i\mathbf{e}_i = \sum_{j=1}^{N} b_i\mathbf{f}_i. \tag{2.15}$$

Computing the inner product,

$$\langle \mathbf{v}, \mathbf{v} \rangle = \sum_{j=1}^{N} (a_j \mathbf{e}_j)^\dagger \sum_{k=1}^{N} a_k \mathbf{e}_k$$

$$= \sum_{j=1}^{N} \sum_{k=1}^{N} \overline{a_j} a_k \underbrace{\mathbf{e}_j^\dagger \mathbf{e}_k}_{\delta_{jk}} \tag{2.16}$$

$$= \sum_{j=1}^{N} |a_j|^2$$

and repeating this using the $\{\mathbf{f}_j\}_{j=1}^{N}$ representation,

$$\langle \mathbf{v}, \mathbf{v} \rangle = \sum_{j=1}^{N} (b_j \mathbf{f}_j)^\dagger \sum_{k=1}^{N} b_k \mathbf{f}_k$$

$$= \sum_{j=1}^{N} |b_j|^2 \tag{2.17}$$

and we find $\sum_{j=1}^{N} |a_j|^2 = \sum_{j=1}^{N} |b_j|^2$, so the inner product is invariant under a basis change.

2.7.2   Representation of Linear Operators

Consider a vector space V_N with basis $\{\mathbf{e}_j\}_{j=1}^{N}$. Consider $\mathbf{b}, \mathbf{c} \in V_N$ and an operator $\hat{A}$, such that $\mathbf{c} = \hat{A}\mathbf{b}$. We can find its representation by considering,

$$\mathbb{1}\mathbf{c} = \mathbb{1}\hat{A}\mathbb{1}\mathbf{b}$$

$$\sum j = 1^N \langle \mathbf{e}_j, \mathbf{c} \rangle \mathbf{e}_j = \sum_{j,k=1}^{N} \left(\mathbf{e}_j \mathbf{e}_j^\dagger \right) \hat{A} \left(\mathbf{e}_k \mathbf{e}_k^\dagger \right) \mathbf{b}$$

$$= \sum_{j,k=1}^{N} \mathbf{e}_j \underbrace{\left(\mathbf{e}_j^\dagger \hat{A} \mathbf{e}_k \right)}_{A_{ij}} \underbrace{\left(\mathbf{e}_k^\dagger \mathbf{b} \right)}_{b_k} \tag{2.18}$$

Thus, we find that we can denote the entries of a matrix $\underline{\underline{A}}$ representing a linear operator $\hat{A}$ are $\left(\underline{\underline{A}} \right)_{ij}$. We can denote this representation by,

$$\hat{A} \xrightarrow{\{e\}_{j=1}^{N}} \underline{\underline{A}}. \tag{2.19}$$

2.7.3   Changing Representation of a Vector

Consider a vector $\mathbf{v} \in V_N$, and orthonormal bases $\{\mathbf{e}_j\}_{j=1}^{N}$ and $\{\mathbf{f}_j\}_{j=1}^{N}$. $\mathbf{v}$ can be decomposed as,

$$\mathbf{v} = \sum_{j=1}^{N} a_i \mathbf{e}_i = \sum_{j=1}^{N} b_i \mathbf{f}_i. \tag{2.20}$$

The lth element of the vector is given by,

$$a_l = \langle \mathbf{e}_l, \mathbf{v} \rangle = \sum_{k=1}^{N} b_k \langle \mathbf{e}_l, \mathbf{f}_k \rangle = \sum_{k=1}^{N} \left(\underline{\underline{U}}_{lk} \right) b_k \tag{2.21}$$

where we have found the matrix $(\underline{\underline{U}})_{lk}$ which represents a unitary operator that takes a vector representation from one basis and transforms it into another. We can denote this,

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} = \begin{pmatrix} \langle \mathbf{e}_1, \mathbf{f}_1 \rangle & \cdots & \langle \mathbf{e}_1, \mathbf{f}_N \rangle \\ \langle \mathbf{e}_2, \mathbf{f}_1 \rangle & \cdots & \langle \mathbf{e}_2, \mathbf{f}_N \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{e}_N, \mathbf{f}_1 \rangle & \cdots & \langle \mathbf{e}_N, \mathbf{f}_N \rangle \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix} \tag{2.22}$$

2.7.4 Changing Representation of a Matrix

We can write a linear operator as,

$$\hat{A} = \mathbb{1}\hat{A}\mathbb{1} = \sum_{j,k=1}^{N} A_{jk}\mathbf{e}_j\mathbf{e}_k^\dagger = \sum_{l,m=1} \tilde{A}_{lm}\mathbf{f}_l\mathbf{f}_m^\dagger \tag{2.23}$$

we then find that,

$$A_{jk} = \sum_{l,m=1}^{N} \langle\mathbf{e}_j, \mathbf{f}_l\rangle \tilde{A}_{lm}\langle\mathbf{f}_m, \mathbf{e}_k\rangle. \tag{2.24}$$

Thus, we find that we can change the matrix representation of a linear operator by,

$$\underline{\underline{A}} = \underline{U}\underline{\tilde{A}}\underline{U}^\dagger. \tag{2.25}$$

2.8 Eigenvalue Problems

> **Definition 28: Eigen Equation**
>
> For a linear operator $\hat{A}$, the eigenequation is,
>
> $$\hat{A}\mathbf{u} = \lambda\mathbf{u} \tag{2.26}$$
>
> where λ and $\mathbf{u}$ are the eigenvalue and right eigenvector of $\hat{A}$ respectively, such that $\mathbf{u} \neq \mathbf{0}$.

A left eigenvector will satisfy,

$$\mathbf{v}^\dagger\hat{A} = \lambda\mathbf{v}^\dagger. \tag{2.27}$$

In order to obtain the eigenvalues, we rearrange to get,

$$\left(\hat{A} - \lambda\hat{\mathbb{1}}\right)\mathbf{u} = 0 \tag{2.28}$$

and solve,

$$\det\left(\hat{A} - \lambda\hat{\mathbb{1}}\right) \tag{2.29}$$

which generates a polynomial of degree N, with N solutions for $\lambda in \mathbb{C}$. Each distinct eigenvalue will correspond to a distinct eigenvector. However, if we have a repeated root, we get repeated eigenvectors. For $m > 1$ repeated eigenvectors, there may be up to, but at least 1, m linearly independent eigenvectors corresponding to the degenerate eigenvalue.

2.8.1 Eigenvalues and eigenvectors of Hermitian operators

> **Theorem 5: Eigenvalues of Hermitian Operators**
>
> Consider the eigenvalues $\{\lambda_i\}_{i=1}^N$ and eigenvectors $\{\mathbf{u}\}_{i=1}^N$ of $\hat{A}$. $\forall\hat{A} : \hat{A}^\dagger = \hat{A} \implies \forall i : \lambda_i \in \mathbb{R}$, $\forall i \neq j : \mathbf{u}_i^\dagger\mathbf{u}_j = 0$.

Proof. The eigenvalue equation is given by,

$$\hat{A}\mathbf{u}_i = \lambda_i\mathbf{u}_i. \tag{2.30}$$

Without loss of generality, consider the matrix elements of $\hat{A}$ with respect to two eigenvectors,

$$\mathbf{u}_j^\dagger\hat{A}\mathbf{u}_k = \lambda_k\langle\mathbf{u}_j, \mathbf{u}_k\rangle. \tag{2.31}$$

Using the Hermitian property,

$$\mathbf{u}_j^\dagger\hat{A}\mathbf{u}_k = \mathbf{u}_j^\dagger\hat{A}^\dagger\mathbf{u}_k = \overline{\mathbf{u}_k^\dagger\hat{A}\mathbf{u}_j} = \overline{\lambda_j}\langle\mathbf{u}_j, \mathbf{u}_k\rangle. \tag{2.32}$$

Equating equations (2.31) and (2.32),

$$(\lambda_k - \overline{\lambda}_k)\langle \mathbf{u}_j, \mathbf{u}_k \rangle = 0. \tag{2.33}$$

Let us consider two cases,

1. $k = j$, since $\langle \mathbf{u}_j, \mathbf{u}_j \rangle > 0$, we require $\lambda_j = \overline{\lambda}_j$.

2. $k \neq j$, since λ_j, λ_k are distinct, we require $\langle \mathbf{u}_j, \mathbf{u}_k \rangle = 0$.

□

2.8.2   Diagonalisation

Let $\underline{U}$ be the matrix with orthonormal eigenvectors $\mathbf{u}_j$ as columns, such that $U_{ij} = (u_j)_i$, and $\hat{U}$ be the corresponding linear operator. By orthogonality, $\hat{U}$ is unitary. For a linear operator $\hat{A}$, we can diagonalise it (construct a matrix with $\hat{A}$'s eigenvalues on the diagonal) by,

$$\left[\hat{U}^\dagger \hat{A} \hat{U}\right]_{ij} = \lambda_i \delta_{ij}. \tag{2.34}$$

To obtain the original operator form its diagonalised form Λ_{ij}, we perform,

$$A_{ij} = U_{ik}\Lambda_{kl}\overline{U}_{jl}. \tag{2.35}$$

Eigenvalues and eigenvectors of unitary operators

We use unitary operators in physics to describe time evolution in quantum mechanics. We can do this because they preserve the norm, and thus the inner product, of a vector. i.e., $\langle \hat{U}\mathbf{u}, \hat{U}\mathbf{v} \rangle = \langle \mathbf{u}, \mathbf{v} \rangle$.

Theorem 6: Eigenvalues of unitary operators

Consider a unitary operator $\hat{U} : V \to V$ with eigenvalue equation,

$$\hat{U}\mathbf{u}_j = \lambda_j \mathbf{u}_j. \tag{2.36}$$

The eigenvalues satisfy the following condition:

1. $|\lambda_j| = 1 \implies \lambda_j = e^{i\theta_j}, \theta \in \mathbb{R}$.

2. $\lambda_j \neq \lambda_k \implies \langle \mathbf{u}_j, \mathbf{u}_k \rangle = 0$.

3. The eigenvectors of $\hat{U}$ form an orthonormal basis for V.

Proof.   1. We need to prove that $|\lambda_j|^2 = 1$. Consider the left anr right eigenequations of $\hat{U}$,

$$\hat{U}\mathbf{u}_j = \lambda\mathbf{u}_j \tag{2.37}$$
$$\mathbf{u}_j^\dagger \hat{U}^\dagger = \overline{\lambda_j}\mathbf{u}_j^\dagger \tag{2.38}$$

from which we find,

$$\begin{aligned}
\mathbf{u}_j^\dagger \hat{U}^\dagger \hat{U} \mathbf{u}_j = \mathbf{u}^\dagger \hat{\mathbb{1}} \mathbf{u} &= \overline{\lambda}\lambda \mathbf{u}_j^\dagger \mathbf{u}_j \\
&= \mathbf{u}^\dagger \mathbf{u} = |\lambda|^2 \mathbf{u}_j^\dagger \mathbf{u} \\
&\implies \left(1 - |\lambda|^2\right)\mathbf{u}_j^\dagger \mathbf{u}_j
\end{aligned} \tag{2.39}$$

we have $\mathbf{u} \neq \mathbf{0}$, so we require $|\lambda|^2 = 1$, and thus $\lambda = e^{i\theta}, \theta \in \mathbb{R}$.

2. Let us consider the left and right eigenequations again. We have,

$$\begin{aligned}
\mathbf{u}_j^\dagger \mathbf{u}_k &= \overline{\lambda_j}\lambda_k \mathbf{u}_j^\dagger \mathbf{u}_k \\
\implies \langle \mathbf{u}_j, \mathbf{u}_k \rangle(1 - \overline{\lambda_j}\lambda_k) &= 0
\end{aligned} \tag{2.40}$$

we require $\overline{\lambda_j}\lambda_k \neq 1, \forall j \neq k, \therefore \langle \mathbf{u}_j, \mathbf{u}_k \rangle$.

3. For completeness, we must write $\mathbf{v} = \sum_{j=1}^{N} c_j \mathbf{u}_j$. We have shown $\{\mathbf{u}_j\}_{i=1}^{N}$ to be orthonormal, so we can write, $c_j = \langle \mathbf{u}_j, \mathbf{v} \rangle$.

□

Spectral Representation

We can diagonalise a general operator $\hat{A}$ which is not necessarily Hermitian, under the assumption that it has a complete set of eigenvectors. The left and right eigenvector equations are,

$$\mathbf{v}_j^\dagger \hat{A} = \lambda_j \mathbf{v}_j^\dagger \qquad\qquad \hat{A}\mathbf{u}_j = \lambda_j \mathbf{u}_j. \tag{2.41}$$

We then have,

$$\mathbf{v}_j^\dagger \hat{A}\mathbf{u}_k = \lambda_k \langle \mathbf{v}_j, \mathbf{u}_k \rangle = \lambda_j \langle \mathbf{v}_j, \mathbf{u}_k \rangle \tag{2.42}$$

thus for $\lambda_j \neq \lambda_k$, we require $\langle \mathbf{v}_j, \mathbf{u}_k \rangle = 0$.

We choose a normalisation $\langle \mathbf{v}_j, \mathbf{u}_k \rangle$, the completeness relation is given by,

$$\sum_{j=1}^N \mathbf{u}_j \mathbf{v}_j^\dagger = \hat{\mathbb{1}} \tag{2.43}$$

and we call $\mathbf{v}_j$ the dual basis to $\mathbf{u}_j$. We can thus write the operator $\hat{A}$,

$$\boxed{\hat{A} = \hat{A}\hat{\mathbb{1}} = \sum_{j=1}^N \hat{A}\mathbf{u}_j \mathbf{v}_j^\dagger = \sum_{j=1}^N \lambda_j \mathbf{u}_j \mathbf{v}_j^\dagger} \tag{2.44}$$

which is known as the *spectral representation* of $\hat{A}$. Given an orthonormal basis $\{\mathbf{e}_j\}_{j=1}^N$ in which we can write the matrix representation of $\hat{A}$ which we denote $\underline{\underline{A}}$, we can diagonalise it by applying,

$$\underline{\underline{A}}^{\text{diag}} = \underline{\underline{S}}\,\underline{\underline{A}}\,\underline{\underline{T}}^\dagger \tag{2.45}$$

where we define,

$$\left(\underline{\underline{S}}\right)_{jk} = \langle \mathbf{v}_j, \mathbf{e}_k \rangle \qquad\qquad \left(\underline{\underline{T}}\right)_{jk} = \langle \mathbf{u}_j, \mathbf{e}_k \rangle \tag{2.46}$$

which are unitary only if $\hat{A}$ is Hermitian.

Diagonalisation of commuting operators

For two commuting operators $\hat{A}$ and $\hat{B}$, when,

$$\hat{B}\mathbf{u} = \lambda \mathbf{u} \tag{2.47}$$

we have,

$$\hat{A}\hat{B}\mathbf{u} = \lambda \hat{A}\mathbf{u}$$
$$\implies \hat{B}\hat{A} = \lambda\left(\hat{A}\mathbf{u}\right) \tag{2.48}$$

and thus $\hat{A}\mathbf{u}$ is also an eigenvector of $\hat{B}$ with eigenvalue λ. Below the implications of this statement are stated,

- **Non-degenerate:** If λ is non-degenerate, $\forall \lambda, \exists \mathbf{u} : \hat{A}\mathbf{u} = \mu\mathbf{u} \implies \mathbf{u}$ is a simultaneous eigenvector of $\hat{B}$ and $\hat{A}$.

- **Degenerate:** If λ has degeneracy $m > 1$, with eigenvectors $\{\mathbf{u}_j\}_{j=1}^m$, then a linear combination of these eigenvectors is an eigenvector of $\hat{A}$. $\hat{B}$ will act in this subspace, and it is possible to find a basis which simultaneously diagonalises $\hat{A}$ and $\hat{B}$.

2.9 Functions of Operators

We wish to apply functions such as $\exp\left(\hat{A}\right)$ to linear operators, and more generally functions such as f.

2.9.1 Taylor Expansion about 0

We have well defined multiplication and addition on operators, so we can construct a Taylor series to define a function of an operator in most cases.

Definition 29: $f(\hat{A})$

For $f : \mathbb{C} \to \mathbb{C}$, with a Taylor series about 0,

$$f(z) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} z^n \tag{2.49}$$

we define the composition of the function and an operator $\hat{A}$ by the same series,

$$f(\hat{A}) = \sum_{n=0}^{\infty} \frac{f^{(0)}}{n!} \hat{A}^n. \tag{2.50}$$

where,

$$f^{(n)}(0) = \left. \frac{\mathrm{d}^n f(0)}{\mathrm{d}x^n} \right|_0 \qquad\qquad \hat{A}^n = \underbrace{\hat{A}\hat{A}\ldots\hat{A}}_{n \text{ times}} \tag{2.51}$$

2.9.2   Spectral Decomposition

Given $\hat{A}$ is diagonalisable, let us apply $f(\hat{A})$ to an eigenvector $\mathbf{u}$ of $\hat{A}$ with eigenvalue λ, assuming f has a Taylor series,

$$\begin{aligned}
f(\hat{A})\mathbf{u} &= \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^n \mathbf{u} \\
&= f(0)\mathbf{u} + \sum_{n=1}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^{n-1} \lambda^n \mathbf{u} \\
&= \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \lambda^n \mathbf{u} = f(\lambda)\mathbf{u}.
\end{aligned} \tag{2.52}$$

If the eigenbasis of $\hat{A}$ is complete, we are able to work in it to represent $f(\hat{A})$ as,

$$f(\underline{\underline{A}}) = \mathrm{diag}\left(\{f(\lambda_j)\}_{j=1}^N\right) \tag{2.53}$$

where diag is a function which constructs a matrix with the values in its arguments on the diagonal, and 0s in all other elements. We can then construct the final operator,

$$f(\hat{A}) = \sum_{i=1}^{N} f(\lambda_i) f(\lambda_i) \mathbf{u}_i \mathbf{v}_i^\dagger \tag{2.54}$$

where $\mathbf{v}_i^\dagger = \mathbf{u}_i^\dagger$ for a Hermitian operator.

2.9.3   Time Evolution Operator

Theorem 7: Unitary operators as exponentials

For a Hermitian operator $\hat{A}$, then,

$$\hat{U}(\theta) = \exp\left(-i\hat{A}\theta\right) \tag{2.55}$$

where $\theta \in \mathbb{R}$, is also unitary.

Proof. Considering the spectral representation of $\hat{A}$, with eigenvalues λ_j and eigenvectors $\mathbf{u}_j$, such that $\hat{A} = \sum_{j=1}^N \lambda_j \mathbf{u}_j \mathbf{u}_j^\dagger$ then,

$$\hat{U}(\theta) = \sum_{j=1}^{N} \exp(-i\lambda_j\theta) \mathbf{u}_j \mathbf{u}_j^\dagger. \tag{2.56}$$

The adjoint $\hat{U}^\dagger(\theta)$ is,

$$\hat{U}^\dagger(\theta) = \sum_{j=1}^N \exp(i\lambda_j\theta)\mathbf{u}_j\mathbf{u}_j^\dagger \tag{2.57}$$

we then find,

$$\hat{U}^\dagger(\theta)\hat{U}(\theta) = \sum_{j,k} e^{-i(\lambda_j-\lambda_k)\theta}\mathbf{u}_k\mathbf{u}_k^\dagger\mathbf{u}_j\mathbf{u}_j^\dagger = \sum_{jk} e^{-i(\lambda_j-\lambda_k)\theta}\mathbf{u}_k^\dagger\langle\mathbf{u}_k,\mathbf{u}_j\rangle\mathbf{u}_j$$
$$= \sum_{jk} e^{-i(\lambda_j-\lambda_k)\theta}\mathbf{u}_k^\dagger\delta_{kj}\mathbf{u}_j = \sum_j \mathbf{u}_j\mathbf{u}_j^\dagger = \hat{\mathbb{1}}. \tag{2.58}$$

thus the operator is unitary. $\qquad\qquad\square$

Furthermore, the operator in equation (2.55) is the time-evolution operator in quantum mechanics, where we would replace $\hat{A}$ with $\hat{H}$ and θ with t.

2.9.4   Overlap Matrix

We wish to develop an alternative method to the Gram-Schmidt process, and will allow us to generalise some things. Let us suppose we have a set of vectors $\{\mathbf{v}_j\}_{j=1}^M$ in a vector space V_N. We will **not** assume that $M \le N$. The matrix overlap is given by,

$$\hat{N} = \sum_{i=1}^M \mathbf{v}_i\mathbf{v}_i^\dagger \tag{2.59}$$

which is Hermitian, and whose matrix representation can be written,

$$N_{kl} = \sum_{i=1}^M v_{ik}\overline{v}_{il}. \tag{2.60}$$

If we are given normalised eigenvectors $\mathbf{u}$ and eigenvalues of $\hat{N}$, we find,

$$\mathbf{u}_k^\dagger\hat{N}\mathbf{u}_k = \lambda_k = \sum_{i=1}^N |\langle\mathbf{v}_i,\mathbf{u}_k\rangle|^2 \ge 0 \tag{2.61}$$

so, all of its eigenvalues must be either positive or 0. If all eigenvalues are positive, we find the inverse of the overlap matrix by writing it in the orthonormal basis $\{\mathbf{u}_j\}_{j=1}^M$,

$$\hat{N}^{-1} = \sum_{i=1}^M \lambda_i^{-1}\mathbf{u}_i\mathbf{u}_i^\dagger. \tag{2.62}$$

For the case that we have a zero eigenvalue, we can define a *pseudo-inverse*.

Definition 30: Pseudo-inverse

For a Hermitian operator $\hat{N}$ with a set of eigenvalues $\{\lambda_i\}_{i=1}^M$ and a set of normalised eigenvectors $\{\mathbf{u}\}_{i=1}^M$, the pseudo-inverse is defined,

$$\hat{N}_+^{-1} = \sum_{i=1}^{M'} \frac{1}{\lambda_i^+}\mathbf{u}_i\mathbf{u}_i^\dagger \tag{2.63}$$

where $\{\lambda_{i,+}\}_{i=1}^{M'} \subset \{\lambda_i\}_{i=1}^M$ containing only the positive eigenvalues of $\hat{N}$, with size $M' < M$.

We can now extract an orthonormal basis from $\mathbf{v}$. We define the inverse square root operator of the overlap matrix as,

> **Definition 31: Inverse square root operator**
>
> $$\hat{N}_+^{-1/2} = \sum_{i=1}^{M'} \frac{1}{\sqrt{\lambda^+}} \mathbf{u}_i \mathbf{u}_i^\dagger. \tag{2.64}$$

If there is a basis, we must have N non-zero eigenvalues, so $M' = N$. We clearly see,

$$\mathbf{e}_i = \hat{N}_+^{-1/2} \mathbf{v}_i \tag{2.65}$$

are orthonormal vectors, and can be used as an N-dimensional basis. We can then find the matrix representation of any operator in this basis, where it is given in a representation $\hat{A} \xrightarrow{\{\mathbf{v}_i\}_i^M} \underline{\underline{A}}$ and $\{\mathbf{v}_i\}_i^M$ is a non-basis, as,

$$\underline{\underline{\tilde{A}}} = \underline{\underline{N_+^{-1/2}}}\,\underline{\underline{A}}\,\underline{\underline{N_+^{-1/2}}} \tag{2.66}$$

2.10   The Trace

> **Definition 32: The Trace**
>
> Consider an operator $\hat{A}$ which acts on a vector space V_N. For a given orthonormal basis $\{\mathbf{e}_j\}_{j=1}^N$, the trace of $\hat{A}$ is the sum of its diagonal elements,
>
> $$\mathrm{Tr}\left(\hat{A}\right) = \sum_{j=1}^N \mathbf{e}_j^\dagger \hat{A} \mathbf{e}_j. \tag{2.67}$$

The trace is independent of basis. We define several properties of the trace below,

1. *Linearity*: $\mathrm{Tr}\left(\alpha\hat{A} + \beta\hat{B}\right) = \alpha\,\mathrm{Tr}\left(\hat{A}\right) + \beta\,\mathrm{Tr}\left(\hat{B}\right)$.

2. *Commutation*: $\mathrm{Tr}\left(\hat{A}\hat{B}\right) = \mathrm{Tr}\left(\hat{B}\hat{A}\right)$.

3. *Trace of a dyad*: $\mathrm{Tr}\left(\mathbf{v}\mathbf{u}^\dagger\right) = \mathrm{Tr}\left(\mathbf{u}^\dagger\mathbf{v}\right) = \langle \mathbf{u}, \mathbf{v} \rangle$.

4. *Invariance under cyclic permutations*: $\mathrm{Tr}\left(\hat{A}\hat{B}\hat{C}\right) = \mathrm{Tr}\left(\hat{B}\hat{C}\hat{A}\right) = \mathrm{Tr}\left(\hat{C}\hat{A}\hat{B}\right)$.

5. *Conjugate of Trace*: $\overline{\mathrm{Tr}\left(\hat{A}\right)} = \mathrm{Tr}\left(\hat{A}^\dagger\right)$, $\overline{\mathrm{Tr}\left(\hat{A}\hat{B}\hat{C}\right)} = \mathrm{Tr}\left(\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger\right)$.

6. *Spectral trace*: If $\hat{A}$ has a spectral representation with eigenvalues $\{\lambda_i\}_{i=1}^N$, then $\mathrm{Tr}\left(\hat{A}\right) = \sum_{i=1}^N \lambda_i$.

2.11   Operators in Function Space

An operator $\hat{A}$ maps a function $|f\rangle \in \mathcal{F}$ to another function $|g\rangle = \hat{A}|f\rangle \in \mathcal{F}'$, or $\hat{A}\mathcal{F} \to \mathcal{F}'$. An example of an operator in function space is the position operator $\hat{x}$. The eigenvectors of the position operator are,

$$\hat{x}|x\rangle = x|x\rangle. \tag{2.68}$$

For a function f, the following equivalence follows

$$|g\rangle = \hat{x}|f\rangle \xrightarrow{|x\rangle} g(x) = xf(x). \tag{2.69}$$

We can write the spectral decomposition of $\hat{x}$ as,

$$\hat{x} = \int_a^b x|x\rangle\langle x|. \tag{2.70}$$

2.11.1 Differential operators

Differential operators are denotes,

$$|g\rangle = \hat{K}|f\rangle \xrightarrow{|x\rangle} g(x) = \sum_n h_n(x)\frac{\mathrm{d}^n}{\mathrm{d}x^n}f(x) \tag{2.71}$$

where $h_n(x)$ is an arbitrary function of x. It can be shown that differential operators are linear.

2.11.2 Changing representation in continuous vector spaces

Given two orthonormal bases $\{\mathbf{u}_n\}_{n=1}^{\infty}$ and $\{\mathbf{v}_n\}_{m=1}^{\infty}$, a function $f : [a, b] \to \mathbb{R}$ can be represented,

$$|f\rangle = \sum_{n=1}^{\infty} f_n |u_n\rangle = \sum_{m=1}^{\infty} c_m |v_m\rangle \tag{2.72}$$

where,

$$f_N = \langle u_n|f\rangle = \int_a^b \overline{u_n(x)}f(x)\,\mathrm{d}x \qquad\qquad c_m = \langle v_m|f\rangle = \int_a^b \overline{v_n(x)}xf(x)\,\mathrm{d}x \tag{2.73}$$

$$= \langle v_m| \sum_{n=1}^{\infty} f_n |u_m\rangle \tag{2.74}$$

$$= \sum_{n=1}^{\infty} f_n \langle v_m|u_n\rangle \tag{2.75}$$

Continuous Bases

Let us consider a basis $|k\rangle$, $k \in [c, d]$, $\langle k|k'\rangle = \delta(k - k')$, so is orthonormal. We have that,

$$\mathbb{1} = \int_c^d \mathrm{d}k\, |k\rangle\langle k| \tag{2.76}$$

so,

$$\begin{aligned}
|f\rangle &= \int_a^b \mathrm{d}x\, |x\rangle\langle x|f\rangle \\
&= \int_c^d \mathrm{d}x\, f(x)\, |x\rangle \\
&= \int_c^d \mathrm{d}k \int_a^b \mathrm{d}x\, f(x)\, |k\rangle\langle k|x\rangle \\
&= \int_c^d \mathrm{d}k \underbrace{\left(\int_a^b f(x)\langle k|x\rangle\right)}_{\tilde{f}(k)} |k\rangle
\end{aligned} \tag{2.77}$$

2.11.3 Momentum Representation

Let us consider a $a = c = -\infty$ and $b = d = +\infty$ and choose $f \in \mathcal{L}^2(\mathbb{R})$. $|k\rangle$ are the eigenstates of $\hat{k} = -i\hat{D}$ such that,

$$\hat{D} \xrightarrow{|x\rangle} \frac{\mathrm{d}}{\mathrm{d}x}, \tag{2.78}$$

k is orthonormal $\langle k|k'\rangle = \delta(k - k')$, and the eigenequation is,

$$\hat{k}|k\rangle = k|k\rangle. \tag{2.79}$$

Consider an overlap with $|x\rangle$ on equation (2.79),

$$\langle x|\hat{k}|k\rangle = k\langle x|k\rangle \tag{2.80}$$

and by Hermitivity,

$$
\begin{aligned}
\langle k| \hat{k} |x\rangle &= +i\frac{\mathrm{d}}{\mathrm{d}x}\overline{\langle k|x\rangle} \\
&= i\frac{\mathrm{d}}{\mathrm{d}x}\underbrace{\langle x|k\rangle}_{\phi_k(x)}.
\end{aligned}
\tag{2.81}
$$

We then have that,

$$
\frac{\mathrm{d}}{\mathrm{d}x}\phi_k(x) = -ik\phi_k(x)
\tag{2.82}
$$

which we can solve trivially,

$$
\phi_k(x) = \frac{1}{\sqrt{2\pi}}e^{-ikx}.
\tag{2.83}
$$

We then find,

$$
\begin{aligned}
\tilde{f}(x) &= \int_{-\infty}^{\infty}\mathrm{d}k\, f(x)\langle k|x\rangle \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\, f(x)e^{ikx}
\end{aligned}
\tag{2.84}
$$

which we recognise as the Fourier transform!

Multiplication Theorem and Parseval's Lemma

Theorem 8: Multiplication Theorem

$\forall f, g : \mathbb{R} \to \mathbb{C}$ where $\exists \tilde{f}, \tilde{g}$ which are Fourier transforms, then

$$
\int_{-\infty}^{\infty}\overline{f(x)}g(x)\,\mathrm{d}x = \int_{-\infty}^{\infty}\overline{\tilde{f}(k)}\tilde{g}(k)\,\mathrm{d}k\,.
\tag{2.85}
$$

This theorem is a consequence of the fact that the inner product is invariant between k and x, as long as the Fourier transform is normalised.

2.11.4   Operators in Momentum Space

Position Operator

Let us change the representation of the position operator in k-space,

$$
\begin{aligned}
\langle k| \hat{x} |f\rangle &= \int_{-\infty}^{\infty}\langle k| \hat{x} |x\rangle \langle x|f\rangle \,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} x f(x)e^{ikx}\,\mathrm{d}x \\
&= -i\frac{\mathrm{d}}{\mathrm{d}k}\underbrace{\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{ikx}\,\mathrm{d}x\right)}_{\tilde{f}(x)}
\end{aligned}
\tag{2.86}
$$

thus, we find,

$$
\hat{x} \xrightarrow{|k\rangle} -i\frac{\mathrm{d}}{\mathrm{d}k}
\tag{2.87}
$$

so the position and momentum operators switch forms when changing between forms.

2.11.5   Coherent States

The annihilation and creation operators (or ladder operators) are,

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{b} + ib\hat{k}\right) \qquad\qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{b} - ib\hat{k}\right) \tag{2.88}$$

and have the property that $\left[\hat{a}, \hat{a}^\dagger\right] = \mathbb{1}$, $\hat{a}\left|0\right> = 0$, and $n(a^\dagger)^{n-1}\left|0\right> = \hat{a}(\hat{a}^\dagger)^n\left|0\right>$. From the annihilation and creation operators we can form a *coherent state basis*, which is defined,

$$\begin{aligned}
\left|z\right> &= N(z)\exp\left(za^\dagger\right)\left|0\right> \qquad z \in \mathbb{Z} \\
&= N(z)\sum_{n=0}^{\infty}\frac{z^n}{n!}\left(a^\dagger\right)^n\left|0\right>.
\end{aligned} \tag{2.89}$$

Taking the overlap of $\left|z\right>$ with another arbitrary $\left|z'\right>$, we find,

$$\begin{aligned}
\left<z|z'\right> &= \overline{N}(z)N(z')\sum_{n,m=0}^{\infty}\frac{\overline{z}^n}{n!}\frac{z'^m}{m!}\underbrace{\left<0\right|\hat{a}^n\hat{a}^m\left|0\right>}_{\delta_{mn}n!} \\
&= \sum_{n=0}^{\infty}\frac{(\overline{z}z')^n}{n!} = \exp(\overline{z}z').
\end{aligned} \tag{2.90}$$

so we find that the coherent state basis can be normalised, but is not orthogonal. However, we can still use it to represent vectors and operators. The completeness relation follows,

$$\mathbb{1} = \frac{1}{\pi}\int_{-\infty}^{\infty}\left|z\right>\left<z\right|\mathrm{d}^2z \tag{2.91}$$