I.2. Inner product spaces

To define the length or magnitude of a vector, the definition of a vector space must be restricted by adding another operation: the inner (or scalar) product.

Remember the dot product in $\mathbb{R}^3$: $|\vec{A}| = \sqrt{\vec{A}\cdot\vec{A}}$

where
- $\vec{A}\cdot\vec{B} = \vec{B}\cdot\vec{A}$ (symmetry)
- $\vec{A}\cdot\vec{A} \geq 0$, $\vec{A}\cdot\vec{A} = 0$ iff $\vec{A} = 0$ (positive semi-definiteness)
- $\vec{A}\cdot(b\vec{B} + c\vec{C}) = b\vec{A}\cdot\vec{B} + c\vec{A}\cdot\vec{C}$ (linearity)

<u>Defn.</u> A vector space with an inner product is called an <u>inner product space</u>.

Do define an inner product $\langle W|V\rangle$ between vectors $|V\rangle, |W\rangle \in \mathbb{V}$, we demand that it fulfills the following properties:

- $\langle V|W\rangle = \langle W|V\rangle^*$ (skew symmetry, ensures that $\langle V|V\rangle$ is real).
- $\langle V|V\rangle \geq 0$; $\langle V|V\rangle = 0$ iff $|V\rangle = |0\rangle$. (positive semidefiniteness)
- $\langle V|(\alpha|W\rangle + \beta|Z\rangle) = \alpha\langle V|W\rangle + \beta\langle V|Z\rangle$ (linearity)

$$= \langle V|\alpha W + \beta Z\rangle$$

From the first and third of these "axioms" follows

$$\langle \alpha W + \beta Z|V\rangle = \langle V|\alpha W + \beta Z\rangle^* = \alpha^*\langle V|W\rangle^* + \beta^*\langle V|Z\rangle^*$$
$$= \alpha^*\langle W|V\rangle + \beta^*\langle Z|V\rangle.$$ (antilinearity in the first ("bra") factor)

$\Rightarrow$ using a basis to expand, we get $\left(|V\rangle = \sum_i v_i |i\rangle, |W\rangle = \sum_j w_j |j\rangle \right)$

$$\boxed{\langle V|W\rangle = \sum_{i,j} v_i^* w_j \langle i|j\rangle}$$

<u>Defn</u> Two vectors are <u>orthogonal</u> if their inner product vanishes.

<u>Defn</u> $|V| \equiv \sqrt{\langle V|V\rangle}$ is the <u>norm</u> or <u>length</u> of the vector.

A <u>normalized vector</u> has unit norm.

<u>Defn</u> A set of normalized basis vectors that are mutually orthogonal is called an <u>orthonormal basis</u>.

In an orthonormal basis we have

$$\langle i|j\rangle = \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & \text{else} \end{cases}$$

and $\langle V|W\rangle = \sum_{i,j} v_i^* w_j \langle i|j\rangle = \sum_i v_i^* w_i \qquad (\Delta)$

$\Rightarrow \langle V|V\rangle = \sum_i v_i^* v_i = \sum_i |v_i|^2 \geq 0 \quad (0 \text{ iff } v_i = 0 \ \forall i)$

<u>Gram-Schmidt theorem</u> Any basis of linearly independent vectors can be orthonormalized by forming appropriate linear combinations of the basis vectors.

(Proof a little later, after we have acquired more familiarity with inner product)

I.3. Dual spaces and Dirac notation

In an orthonormal basis $\{|i\rangle\}$ we can represent any vector through its components, say in a column vector:

$$|V\rangle \mapsto \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} , \quad |W\rangle \longmapsto \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_2 \end{bmatrix}$$

The inner product (Δ) can then be understood as performing a matrix multiplication between the transpose conjugate of one vector with the other:

$$\langle V|W\rangle = [v_1^*, v_2^*, \ldots, v_n^*] \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

We can thus associate $\langle V|$ with the row vector $[v_1^*, v_2^*, \ldots, v_n^*]$, and vice versa. So, given a "ket" $|V\rangle$, represented in an orthonormal basis $|i\rangle$ as a column vector $\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$.

we can construct a <u>dual "bra" vector</u> $\langle V|$, represented in the (dual version of the) same basis as a row vector $[v_1^*, v_2^*, \ldots, v_n^*]$:

$$|V\rangle = \sum_i v_i |i\rangle \leftrightarrow \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \longleftrightarrow [v_1^*, v_2^*, \ldots, v_n^*] \leftrightarrow \sum_i v_i^* \langle i| = \langle V|$$

"$\leftrightarrow$" means "within a basis".

Obviously, the basis vectors themselves are represented as

$$|i\rangle \leftrightarrow \begin{array}{c} \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \end{array} \begin{array}{l} \\ \\ \leftarrow i^{\text{th}} \text{ row} \\ \\ \\ \end{array} \qquad \langle j| \leftrightarrow \begin{array}{c} [0, \ldots, 1, \ldots, 0] \\ \uparrow j^{\text{th}} \text{ column.} \end{array}$$

The above insights allow us to compute the coefficients of an arbitrary vector $|V\rangle$ in a specific orthonormal basis: $\boxed{v_i = \langle i|V\rangle}$

Proof: If $|V\rangle = \sum_j v_j |j\rangle$, then $\langle i|V\rangle = \sum_j v_j \underbrace{\langle i|j\rangle}_{\delta_{ij}} = v_i$ ✓

Similarly, $\boxed{\langle V|i\rangle = v_i^*}$

$$\left(\langle V| = \sum_j v_j^* \langle j| \Rightarrow \langle V|i\rangle = \sum_j v_j^* \underbrace{\langle j|i\rangle}_{\delta_{ji}} = v_i^*\right)$$

The transition from the column $\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$ to the complex conjugate row $[v_1^*, v_2^*, \dots, v_n^*]$, and vice versa, is called the "adjoint operation"

We therefore also call the bra $\langle V|$ the adjoint of the ket $|V\rangle$, and vice versa. For the adjoint of $a|V\rangle$ we get

$$a|V\rangle \leftrightarrow \begin{bmatrix} av_1 \\ av_2 \\ \vdots \\ av_n \end{bmatrix} \leftrightarrow [a^*v_1^*, a^*v_2^*, \dots, a^*v_n^*] \leftrightarrow \langle V|a^*$$

$\Leftrightarrow \quad \boxed{\langle aV| = \langle V|a^*}$ (the adjoint of $|aV\rangle$ is a^* times the adjoint of $|V\rangle$).

If $a|V\rangle = b|W\rangle + c|Z\rangle$, then $\boxed{\langle aV| = \langle V|a^* = \langle W|b^* + \langle Z|c^*}$

Recalling that $v_i = \langle i|V\rangle$, we can derive

$$\boxed{\begin{aligned} |V\rangle &= \sum_i v_i |i\rangle = \sum_i |i\rangle\langle i|V\rangle \\ \langle V| &= \sum_i v_i^* \langle i| = \sum_i \langle V|i\rangle\langle i| \end{aligned}} \Rightarrow \sum_i |i\rangle\langle i| = \mathbb{1}$$

(basis decomposition of the unit operator)

Proof of the Gram-Schmidt theorem: by construction.

Let $|I\rangle, |II\rangle, \ldots$ be a linearly independent (but not yet orthonormal) basis.

Set $\boxed{|1\rangle \equiv \frac{|I\rangle}{|I|} = \frac{|I\rangle}{\sqrt{\langle I|I\rangle}}}$ (such that $\langle 1|1\rangle = 1$)

For the second vector, consider

$$|2'\rangle = |II\rangle - |1\rangle\langle 1|II\rangle$$ ($= |II\rangle$ minus the part pointing along $|1\rangle$)

$$\Rightarrow \langle 1|2'\rangle = \langle 1|II\rangle - \underbrace{\langle 1|1\rangle}_{1}\langle 1|II\rangle = 0 \qquad (|2'\rangle \perp |1\rangle)$$

Normalize:

$$\boxed{|2\rangle = \frac{|2'\rangle}{|2'|} = \frac{|2'\rangle}{\sqrt{\langle 2'|2'\rangle}} = \frac{|II\rangle - \langle 1|II\rangle|1\rangle}{\sqrt{\langle II|II\rangle - |\langle 1|II\rangle|^2}}}$$

Next:

$$|3'\rangle = |III\rangle - |1\rangle\langle 1|III\rangle - |2\rangle\langle 2|III\rangle$$ (which is $\perp$ to both $|1\rangle$ and $|2\rangle$)

and $|3\rangle = \dfrac{|3'\rangle}{\sqrt{\langle 3'|3'\rangle}}$

etc. etc.

Linear independence of the original set ensures that this procedure never stops (by obtaining for $|i'\rangle$ the null vector) until we arrive at $|n\rangle$.

Example: Orthonormalize the vectors $|I\rangle = \begin{pmatrix}3\\0\\0\end{pmatrix}$, $|II\rangle = \begin{pmatrix}0\\1\\2\end{pmatrix}$, $|III\rangle = \begin{pmatrix}0\\2\\5\end{pmatrix}$

Solution: $|I\rangle$ is already normal to $|II\rangle$ and $|III\rangle$. So we only need to normalize $|I\rangle$ and $|II\rangle$ and then orthonormalize $|III\rangle$ to $|II\rangle$.

$$\Rightarrow \boxed{|1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}, \quad |2\rangle = \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}}$$

$$|3'\rangle = |III\rangle - |1\rangle\underbrace{\langle 1|III\rangle}_{0} - |2\rangle\langle 2|III\rangle = \begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}\underbrace{\left(1, 1/\sqrt{5}, 2/\sqrt{5}\right)\begin{pmatrix}0\\2\\5\end{pmatrix}}_{\frac{12}{\sqrt{5}}}$$

$$= \begin{pmatrix}0 - 0\\2 - \frac{12}{5}\\5 - \frac{24}{5}\end{pmatrix} = \begin{pmatrix}0\\-2/5\\+1/5\end{pmatrix} \Rightarrow \boxed{|3\rangle = \begin{pmatrix}0\\-1/\sqrt{5}\\+2/\sqrt{5}\end{pmatrix}}$$

(**Note**: Gram-Schmidt does not give $\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}$! In general, if you relabel the original vectors (i.e. orthonormalize them in different order), you get different orthonormal bases.)

Schwarz inequality: Thm: $|\langle V|W\rangle| \leq |V|\cdot|W|$

(or $\langle V|W\rangle\langle W|V\rangle \leq \langle V|V\rangle\langle W|W\rangle$)

(trivial for vectors in $\mathbb{R}^3$: $|\vec{V}\cdot\vec{W}| = |V||W||\cos\vartheta| \leq |V||W|$)

Proof: Consider $|Z\rangle = |V\rangle - \frac{\langle W|V\rangle}{|W|^2}|W\rangle$

$$0 \leq \langle Z|Z\rangle = \left(\langle V| - \frac{\langle W|V\rangle^*}{|W|^2}\langle W|\right)\left(|V\rangle - \frac{\langle W|V\rangle}{|W^2|}|W\rangle\right)$$

$$= \langle V|V\rangle - \frac{\langle W|V\rangle^*\langle W|V\rangle}{|W|^2} - \frac{\langle W|V\rangle\langle V|W\rangle}{|W|^2} + \frac{\langle W|V\rangle^*\langle W|V\rangle}{|W|^2}\langle W|V\rangle$$

$$= \langle V|V\rangle - \frac{|\langle W|V\rangle|^2}{|W|^2} \quad \diamond$$

Triangle inequality: Thm: $|V+W| \leq |V| + |W|$

Proof: homework

I.4. Subspaces

Defn A subset of elements of a vector space $\mathbb{V}$, that form a vector space among themselves, is called a subspace. If subspace i has dimension n_i we denote it as $\mathbb{V}_i^{n_i}$.

Examples in $\mathbb{R}^3 \equiv \mathbb{V}^3(\mathbb{R})$

$\mathbb{V}_x^1$ = all vectors along x axis

$\mathbb{V}_y^1$ = all vector along y axis

$\mathbb{V}_{xy}^2$ = all vectors in xy plane

All subspaces contain the null vector $|0\rangle$, and with each vector of a subspace its additive inverse is also in the subspace.

Defn: The sum of two subspaces $\mathbb{V}_i^{n_i}$ and $\mathbb{V}_j^{m_j}$, denoted as $\mathbb{V}_i^{n_i} \oplus \mathbb{V}_j^{m_j}$, contains all linear combinations of vectors in $\mathbb{V}_i^{n_i}$ and $\mathbb{V}_j^{m_j}$.

Exercise (homework) Prove that in a vector space $\mathbb{V}^n$, the set of all vectors orthogonal to a given vector $|V\rangle \neq 0$ forms a subspace $\mathbb{V}_\perp^{n-1}$ of dimension $n-1$.

1.5 Linear Operators

An operator $\hat{\Omega}$ is an instruction for transforming any vector $|V\rangle \in \mathbb{V}$ into another $|V'\rangle \in \mathbb{V}$:

$$\hat{\Omega}|V\rangle = |V'\rangle$$

Operators can also act on bras:

$$\langle V'|\hat{\Omega} = \langle V''|$$

Consider only linear operators that satisfy

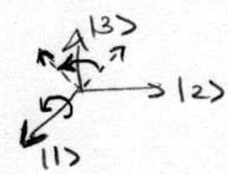
$$\hat{\Omega}\Big(\alpha|V\rangle + \beta|W\rangle\Big) = \alpha\hat{\Omega}|V\rangle + \beta\hat{\Omega}|W\rangle$$

$$\Big(\langle V|\alpha + \langle W|\beta\Big)\hat{\Omega} = \alpha\langle V|\hat{\Omega} + \beta\langle W|\hat{\Omega}$$

Examples
- Identity operator $\hat{I}$: $\left.\begin{array}{l}\hat{I}|V\rangle = |V\rangle \\ \langle V|\hat{I} = \langle V|\end{array}\right\} \forall |V\rangle$

- $\hat{R}(\frac{\pi}{2}\vec{e}_1)$ on $\mathbb{V}^3(\mathbb{R})$: rotate vector by $\frac{\pi}{2}$ around unit vector $\vec{e}_1$

Denote $\vec{e}_1, \vec{e}_2, \vec{e}_3$ as $|1\rangle, |2\rangle, |3\rangle$.



$$\Rightarrow \hat{R}(\tfrac{\pi}{2}\vec{e}_1)\,|1\rangle = |1\rangle$$
$$\hat{R}(\tfrac{\pi}{2}\vec{e}_1)\,|2\rangle = |3\rangle$$
$$\hat{R}(\tfrac{\pi}{2}\vec{e}_1)\,|3\rangle = -|2\rangle$$
$$\hat{R}(\tfrac{\pi}{2}\vec{e}_1)\big(|2\rangle + |3\rangle\big) = |3\rangle - |2\rangle = \hat{R}|2\rangle + \hat{R}|3\rangle$$

Once we know the action of a linear operator $\hat{\Omega}$ on the basis states $\{|i\rangle\}$, we know its action on all vectors:

$$\hat{\Omega}|V\rangle = \hat{\Omega}\sum_i v_i|i\rangle = \sum_i v_i\,\hat{\Omega}|i\rangle = \sum_i v_i\,|i'\rangle$$

Product of two operators = sequential operations:

$$\hat{\Lambda}\hat{\Omega}|V\rangle = \hat{\Lambda}\left(\hat{\Omega}|V\rangle\right) = \hat{\Lambda}|\hat{\Omega}V\rangle$$

In general the order matters, i.e.

$$\underbrace{[\hat{\Omega},\hat{\Lambda}]}_{} = \hat{\Omega}\hat{\Lambda} - \hat{\Lambda}\hat{\Omega} \neq 0 \iff \hat{\Omega}|\hat{\Lambda}V\rangle \neq \hat{\Lambda}|\hat{\Omega}V\rangle$$

commutator of $\hat{\Omega}$ and $\hat{\Lambda}$, $[\hat{\Omega},\hat{\Lambda}] = -[\hat{\Lambda},\hat{\Omega}]$

Example: $\frac{\pi}{2}$ rotations around $\vec{e}_1$ and $\vec{e}_2$ in $\mathbb{V}^3(\mathbb{R})$ don't commute.

Useful identities:

$$\boxed{\begin{aligned} [\hat{\Omega},\hat{\Lambda}\hat{\theta}] &= \hat{\Lambda}[\hat{\Omega},\hat{\theta}] + [\hat{\Omega},\hat{\Lambda}]\hat{\theta} \\ [\hat{\Lambda}\hat{\Omega},\hat{\theta}] &= \hat{\Lambda}[\hat{\Omega},\hat{\theta}] + [\hat{\Lambda},\hat{\theta}]\hat{\Omega} \end{aligned}}$$

$\left(= \cancel{\hat{\Lambda}\hat{\Omega}\hat{\theta}} - \hat{\Lambda}\hat{\theta}\hat{\Omega} + \hat{\Omega}\hat{\Lambda}\hat{\theta} - \cancel{\hat{\Lambda}\hat{\Omega}\hat{\theta}}\right)$

$\left(= \hat{\Lambda}\hat{\Omega}\hat{\theta} - \cancel{\hat{\Lambda}\hat{\theta}\hat{\Omega}} + \cancel{\hat{\Lambda}\hat{\theta}\hat{\Omega}} - \hat{\theta}\hat{\Lambda}\hat{\Omega}\right)$

The <u>inverse</u> of $\hat{\Omega}$, denoted by $\hat{\Omega}^{-1}$, satisfies

$$\hat{\Omega}\hat{\Omega}^{-1} = \hat{\Omega}^{-1}\hat{\Omega} = \hat{I}$$

The inverse exists if $\hat{\Omega}|V\rangle = |0\rangle$ implies $|V\rangle = |0\rangle$.

The inverse of $\hat{\Omega}\hat{\Lambda}$ is $(\hat{\Omega}\hat{\Lambda})^{-1} = \hat{\Lambda}^{-1}\hat{\Omega}^{-1}$.

$$\left((\hat{\Omega}\hat{\Lambda})(\hat{\Omega}\hat{\Lambda})^{-1} = \hat{\Omega}\hat{\Lambda}\hat{\Lambda}^{-1}\hat{\Omega}^{-1} = \hat{\Omega}\hat{\Omega}^{-1} = \hat{I} \right)$$

I.6. Matrix elements of linear operators

As stated, to know how $\hat{\Omega}$ acts on any $|V\rangle$, we only need to know its action on the basis:

$$\hat{\Omega}|i\rangle = |i'\rangle \qquad (i = 1, 2, \ldots, n)$$

We know this action if we know the components of $|i'\rangle$ in the basis $\{|i\rangle\}$:

$$\langle j|i'\rangle = \langle j|\hat{\Omega} i\rangle = \langle j|\hat{\Omega}|i\rangle \equiv \Omega_{ji}$$

The n^2 number Ω_{ji} are the matrix elements of $\hat{\Omega}$ in this basis.

Then $\hat{\Omega}|V\rangle = |V'\rangle$

where $|V'\rangle$ has the components

$$v_i' = \langle i|V'\rangle = \langle i|\hat{\Omega}|V\rangle = \langle i|\hat{\Omega} \sum_j v_j|j\rangle)$$
$$= \sum_j \langle i|\hat{\Omega}|j\rangle v_j = \sum_i \Omega_{ij} v_j$$

This can be written in matrix form:

$$\begin{bmatrix} v_1' \\ v_2' \\ \vdots \\ \vdots \\ v_n' \end{bmatrix} = \begin{bmatrix} \Omega_{11} & \Omega_{12} & \cdots & \Omega_{1n} \\ \Omega_{21} & & & \vdots \\ \vdots & & & \vdots \\ \Omega_{n1} & \cdots & \cdots & \Omega_{nn} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ \vdots \\ v_n \end{bmatrix}$$

The j^{th} column are given by the image of the j^{th} basis vector $|j\rangle$ after $\hat{\Omega}$ acts on it.

Example $\hat{R} \equiv \hat{R}(\frac{\pi}{2}\vec{e}_1)$

$$\begin{aligned} \hat{R}\,|1\rangle &= |1\rangle \\ \hat{R}\,|2\rangle &= |3\rangle \\ \hat{R}\,|3\rangle &= |-2\rangle \end{aligned} \Rightarrow [R_{ij}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

Exercise: How can you describe the action of (Homework) $\hat{\Omega}$ whose matrix elements in the same basis are given by $\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$?

Matrix forms of some specific operators

(1) Identity operator: $I_{ij} = \langle i|\hat{I}|j\rangle = \langle i|j\rangle = \delta_{ij} \leftrightarrow \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}$

(2) Projection operators:

Consider the expansion of an arbitrary ket $|V\rangle$ as

$$|V\rangle = \sum_{i=1}^{n} |i\rangle\langle i|V\rangle = \left(\sum_{i=1}^{n} |i\rangle\langle i|\right)|V\rangle$$

Since this is true for all $|V\rangle$, the expression in brackets must be the identity operator:

$$\hat{I} = \sum_{i=1}^{n} |i\rangle\langle i| \equiv \sum_{i=1}^{n} \hat{\mathbb{P}}_i \qquad (*)$$

The object $\hat{\mathbb{P}}_i = |i\rangle\langle i|$ is called the projection operator for the ket $|i\rangle$. Eq. (*) is called completeness relation, it expresses the identity operator as a sum over projection operators. This will prove very valuable.