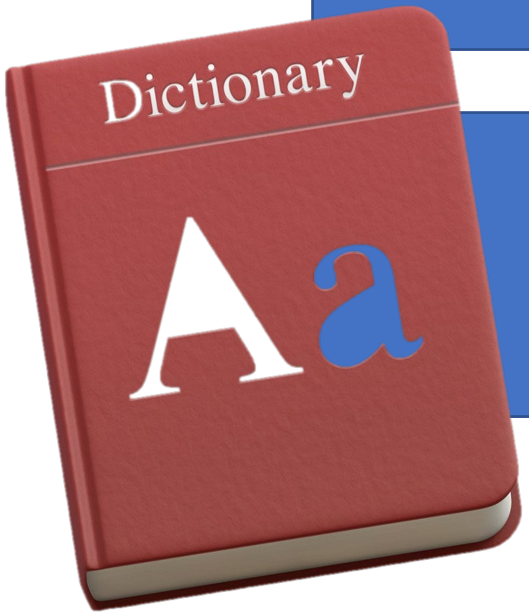
1. The mathematical language: Linear Algebra



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Hilbert spaces

A Hilbert space $\mathcal{H}$ is a **linear vector space** over the field $\mathbb{C}$ possessing an inner product which induces a norm and is complete with respect to this norm.

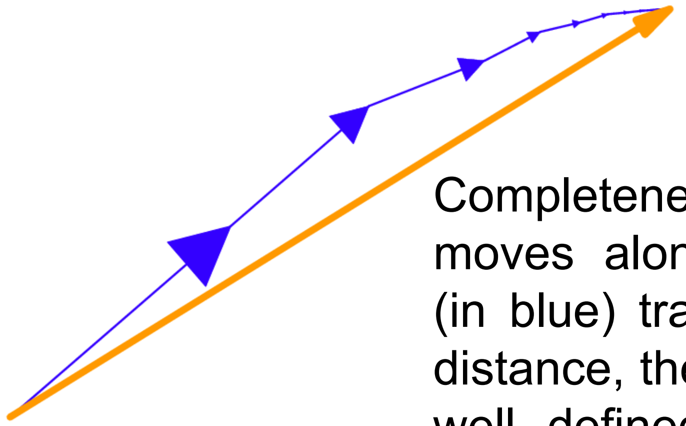
We use hereafter **Dirac notation**.

Linear superpositions of vectors still belong to $\mathcal{H}$ $\quad |v\rangle, |w\rangle \in \mathcal{H} \Rightarrow \alpha|v\rangle + \beta|w\rangle \in \mathcal{H}$

Inner product: $\langle v|w\rangle \in \mathbb{C}$
linear map associating a complex number to each pair of elements $|v\rangle, |w\rangle \in \mathcal{H}$. Given $\alpha, \beta \in \mathbb{C}$ the following **properties** hold

- $\langle v|(\alpha|w_1\rangle + \beta|w_2\rangle) = \alpha\langle v|w_1\rangle + \beta\langle v|w_2\rangle$
- $\langle v|w\rangle = \langle w|v\rangle^*$
- $\langle v|v\rangle \geq 0$
- $\langle v|v\rangle = 0$ if and only if $|v\rangle = 0$

We then define the norm of state $|v\rangle$ as $\|v\| = \sqrt{\langle v|v\rangle}$.



Completeness: if a particle moves along the broken path (in blue) travelling a finite total distance, then the particle has a well defined net displacement (in orange)

Bra-kets and vectors

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \quad \Rightarrow \quad \langle v| = |v\rangle^\dagger = (v_1^* \quad v_2^* \quad \cdots \quad v_n^*)$$

$$|w\rangle = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix}$$

Inner product $$\langle v|w\rangle = (v_1^* \quad v_2^* \quad \cdots \quad v_n^*)\begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = v_1^* w_1 + v_2^* w_2 + \cdots + v_n^* w_n$$

Norm $$\||v\rangle\| = \sqrt{\langle v|v\rangle} = \sqrt{|v_1|^2 + |v_2|^2 + \cdots |v_n|^2}$$

Orthonormal basis sets

Two vectors $|v\rangle, |w\rangle \in \mathcal{H}$ are orthogonal if $\langle v|w\rangle = 0$.

Given a subspace $A \subseteq \mathcal{H}$, its orthogonal complement $A^\perp$ is the set of all vectors orthogonal to A.

If A is closed, the Hilbert space $\mathcal{H}$ is the direct sum of the two complementary closed spaces A and $A^\perp$, i.e. $\mathcal{H} = A \oplus A^\perp$ (Beppo-Levi theorem).

A set $U \subset \mathcal{H}$ of orthonormal vectors $|u_k\rangle$ (orthogonal and with unit norm) is complete if

$$\boxed{\sum_k |u_k\rangle\langle u_k| = \mathbb{I}} \qquad \text{i.e.} \qquad |v\rangle = \sum_k \langle u_k|v\rangle |u_k\rangle \quad \forall |v\rangle \in \mathcal{H}$$

COMPLETENESS RELATION

Therefore, U is a "good" basis set for $\mathcal{H}$. The size of U is the dimension of the Hilbert space.

Examples ($d = 2$)

$$U = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \quad \Rightarrow \quad \begin{pmatrix} a \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |v\rangle$$

$$U = \left\{ \underbrace{\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}}_{u_0}, \underbrace{\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}}_{u_1} \right\}$$

$$\langle u_0|v\rangle = \frac{a+b}{\sqrt{2}} \qquad \langle u_1|v\rangle = \frac{a-b}{\sqrt{2}}$$

$$|v\rangle = \frac{a+b}{\sqrt{2}} |u_0\rangle + \frac{a-b}{\sqrt{2}} |u_1\rangle$$

Linear Operators and matrices

Linear operator $A\colon \mathcal{H} \to \mathcal{H}$ $\quad A(\alpha|v\rangle + \beta|w\rangle) = \alpha A|v\rangle + \beta A|w\rangle$

Limited if $\exists M \in \mathbb{R}$ s.t. $\||A|v\rangle\| \le M\||v\rangle\| \;\; \forall |v\rangle \in \mathcal{H}$ Then $\|A\| \doteq \sup_{|v\rangle \neq 0} \dfrac{\|A|v\rangle\|}{\||v\rangle\|}$

Matrix representation $|w\rangle = A|v\rangle \to |w_i\rangle = \sum_j A_{ij}|v_j\rangle$

Outer product Given $|v\rangle \in V$, $|w\rangle \in W$ Define $U\colon V \to W$

$U = |w\rangle\langle v|$ whose action is defined by $(|w\rangle\langle v|)|v'\rangle = |w\rangle\langle v|v'\rangle = \langle v|v'\rangle|w\rangle$

Recall the **completeness** relation:
given an orthonormal basis set $|k\rangle$ for the Hilbert space $\mathcal{H}$, any vector $|v\rangle \in \mathcal{H}$ can be written as $|v\rangle = \sum_k v_k|k\rangle$, with complex coefficients $v_k = \langle k|v\rangle$. Hence $|v\rangle = \sum_k \langle k|v\rangle|k\rangle = \sum_k |k\rangle\langle k|v\rangle$.
Since this equality holds $\forall|v\rangle$, we get $\boxed{\sum_k |k\rangle\langle k| = \mathbb{I},}$ i.e. the completeness relation.

We can use the completeness relation to obtain the outer product representation of an operator A:

$$A = \mathbb{I}_W A \mathbb{I}_V = \sum_{j,k} |w_j\rangle\langle w_j|A|v_k\rangle\langle v_k| = \sum_{j,k} \langle w_j|A|v_k\rangle |w_j\rangle\langle v_k| = \sum_{j,k} A_{jk}|w_j\rangle\langle v_k|$$

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Some useful operators

Given an operator A acting in the Hilbert space $\mathcal{H}$, there exist a unique operator $A^\dagger$ such that

$$\forall |v\rangle, |w\rangle \in \mathcal{H} \qquad (|v\rangle, A|w\rangle) = \left(A^\dagger|v\rangle, |w\rangle\right)$$

We call $A^\dagger$ the **adjoint** of A.

It is easy to see that $(AB)^\dagger = B^\dagger A^\dagger$. By convention $|v\rangle^\dagger = \langle v| \Rightarrow (A|v\rangle)^\dagger = \langle v|A^\dagger$

In a matrix representation, $A^\dagger = (A^*)^T$

A is **Hermitian** or self-adjoint if $A^\dagger = A$

Let $\{|1\rangle, \dots, |d\rangle\}$ be an orthonormal basis set for the Hilbert space $\mathcal{H}$ of dimension d and let V be a subspace of $\mathcal{H}$ spanned by the orthonormal basis set $\{|1\rangle, \dots, |n\rangle\}$, with $n < d$. Then

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & \\ & & & \ddots \; 0 \end{pmatrix} = P \equiv \sum_{k=1}^{n} |k\rangle\langle k|$$

Is the **projector** onto the subspace V. We can check that it is

- Hermitian ($P^\dagger = P$)
- Idem-potent $P^2 = P$

$$P^2 = \sum_{k,j} |k\rangle\underbrace{\langle k|j\rangle}_{\delta_{kj}}\langle j| = \sum_k |k\rangle\langle k| = P$$

The orthogonal complement of P is the operator $Q = \mathbb{I} - P$. Using the completeness relation, we can check that

$$Q \equiv \sum_{k=n+1}^{d} |k\rangle\langle k| = \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix}$$

The vector space spanned by Q is the orthogonal complement of V.

$$P + Q = \mathbb{I}$$

Some useful operators

Normal operator $A^\dagger A = AA^\dagger$

Unitary operator $U^\dagger U = UU^\dagger = \mathbb{I}$

Unitary operator preserve norm and inner products:

If U is invertible, $U^\dagger = U^{-1}$

$$(U|v\rangle, U|w\rangle) = \langle v|U^\dagger U|w\rangle = \langle v|\mathbb{I}\,|w\rangle = \langle v|w\rangle$$

$$\langle v|U^\dagger U|v\rangle = \langle v|v\rangle$$

Outer product representation (for any two orthonormal basis sets $|u_k\rangle$ and $|v_k\rangle$)

$$U = \sum_k |u_k\rangle\langle v_k|$$

This matrix represents the basis transformation from $|v_k\rangle$ to $|u_k\rangle$

Pauli matrices

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are **Hermitian and unitary**

Eigenvalues and eigenvectors

Eigenvalue equation $A|u\rangle = \lambda|u\rangle$

Complex eigenvalue

Eigenvector

Eigenvalues can be found by solving the characteristic equation. $\det|A - \lambda\mathbb{I}| = 0$
The set of (discrete) eigenvalues λ is the **spectrum** of A.

Hermitian operators are characterized by:

- **real eigenvalues** and
- **eigenvectors** corresponding to different eigenvalues are **orthogonal**

Diagonal (outer product) representation of A (discrete spectrum): $\Lambda = \sum_k \lambda_k P_k = \sum_k \lambda_k |u_k\rangle\langle u_k|$

This is an orthonormal decomposition into orthonormal eigenspaces spanned by eigenvectors $|u_k\rangle$

Given the unitary matrix V whose columns represent the eigenvectors: $\Lambda = V^\dagger A V$

Change of basis: given the unitary matrix $U = \sum_k |u_k\rangle\langle v_k|$ $A_u = U^\dagger A_v U$ Operator A written in the new basis $|u_k\rangle$

Example: Pauli matrices

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad |Z - \lambda\mathbb{I}| = \begin{vmatrix} 1-\lambda & 0 \\ 0 & -1-\lambda \end{vmatrix} = -(1-\lambda)(1+\lambda)$$

$$|Z - \lambda\mathbb{I}| = 0 \Longrightarrow (1-\lambda)(1+\lambda) = 0 \Longrightarrow \lambda = \pm 1 \qquad |u_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |u_{-1}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad |X - \lambda\mathbb{I}| = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1$$

$$|X - \lambda\mathbb{I}| = 0 \Longrightarrow \lambda^2 - 1 = 0 \Longrightarrow \lambda = \pm 1 \qquad |u_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |u_{-1}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The eigenvalues of unitary matrices are complex numbers of modulus 1. Indeed

$$U|\phi\rangle = \lambda|\phi\rangle \Longrightarrow \langle\phi|U^\dagger = \lambda^*\langle\phi| \Longrightarrow \langle\phi|U^\dagger U|\phi\rangle = \lambda^*\lambda \Longrightarrow \lambda^*\lambda = 1$$

$U|\phi\rangle = \lambda|\phi\rangle$ $\qquad \langle\phi|U^\dagger U|\phi\rangle = \langle\phi|\phi\rangle$

$\langle\phi|U^\dagger = \lambda^*\langle\phi|$ $\qquad \lambda^*\lambda\langle\phi|\phi\rangle =$ $\qquad \lambda^*\lambda = 1$

$|\lambda|^2 = 1$

Operator functions

$\sigma_x = X, \sigma_y = Y$

Commutator $[A, B] = AB - BA$ $\qquad [\sigma_\alpha, \sigma_\beta] = 2i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma$

Anti-commutator $\{A, B\} = AB + BA$ $\qquad [X, Y] = XY - YX = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = 2iZ$

Verify the following identities: $\qquad [Z, X] = 2iY$

$$AB = \frac{\{A, B\} + [A, B]}{2} \qquad [A, B]^\dagger = [B^\dagger, A^\dagger] \qquad \{\sigma_\alpha, \sigma_\beta\} = 0$$

$XY + YX = 0$

Simultaneous diagonalization theorem:

$[A, B] = 0 \Leftrightarrow$ there exist a basis of simultaneous eigenvectors for A and B

Trace $\qquad \mathrm{Tr}A = \sum_i A_{ii}$

- Cyclic $\mathrm{Tr}[ABC] = \mathrm{Tr}[CAB] = \mathrm{Tr}[BCA]$
- Linear $\mathrm{Tr}[aA + bB] = a\mathrm{Tr}[A] + \mathrm{b}\mathrm{Tr}[B]$

$$\mathrm{Tr}\,[\mathrm{A}|\psi\rangle\langle\psi|] = \sum_i \langle i|A|\psi\rangle\langle\psi|i\rangle = \underbrace{\sum_i \langle\psi|i\rangle\langle i|}_{=\mathbb{I}} A|\psi\rangle = \langle\psi|A|\psi\rangle$$

Matrix exponential

Given a Hermitian limited operator H, the operator $e^{iHt} = \sum_{n=0}^{\infty} \frac{i^n t^n}{n!} H^n = U$ is unitary.

Indeed, $U^\dagger = e^{-iH^\dagger t} = e^{-iHt}$. Hence $U^\dagger U = e^{-iHt} e^{iHt} = \mathbb{I}$

Pauli matrices $\quad \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$h = a_1 X + a_2 Y + a_3 Z = \begin{pmatrix} a_3 & a_1 - i a_2 \\ a_1 + i a_2 & -a_3 \end{pmatrix}$$

$a_1 = \mathrm{Tr}(Xh)/2 \quad a_2 = \mathrm{Tr}(Yh)/2 \quad a_3 = \mathrm{Tr}(Zh)/2$

$\mathrm{Tr}(h) = 0$

$a_i \in \mathbb{R}$

$$h^2 = a^2 \mathbb{I} \Rightarrow h^{2n} = a^{2n}\mathbb{I}, \quad h^{2n+1} = a^{2n} h \qquad a^2 = a_1^2 + a_2^2 + a_3^2$$

$$\Rightarrow \quad e^{ih} = \sum_{n=0}^{\infty} \frac{(ih)^{2n}}{(2n)!} + \frac{(ih)^{2n+1}}{(2n+1)!} = \sum_{n=0}^{\infty} \frac{(h)^{2n}}{(2n)!}(-1)^n + i \sum_{n=0}^{\infty} \frac{(h)^{2n+1}}{(2n+1)!}(-1)^n$$

$$= \mathbb{I} \underbrace{\sum_{n=0}^{\infty} \frac{(-1)^n a^{2n}}{(2n)!}}_{\cos a} + ih \underbrace{\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} a^{2n}}_{\sin a / a}$$

$$\Rightarrow \quad e^{ih} = \mathbb{I} \cos a + ih \frac{\sin a}{a}$$

Exercise

We can easily find eigenvalues and eigenvectors of the generic Hermitian zero-trace matrix h . These are

$$\lambda_{\pm} = \pm a = \pm\sqrt{a_1^2 + a_2^2 + a_3^2} \qquad |\phi_{\pm}\rangle = \begin{pmatrix} \frac{\pm(a_1 - ia_2)}{\sqrt{2a(a \mp a_3)}} \\ \sqrt{\frac{a \mp a_3}{2a}} \end{pmatrix}$$

The most general Hermitian matrix H of order 2 can be decomposed into Pauli matrices as follows:

Hilbert-Schmidt inner products on operators: $(A, B) = \mathrm{Tr}[A^\dagger B]$

$$H = \begin{pmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{pmatrix}$$

$$a_0 = (\mathrm{I}, \mathrm{H})/\|I\|^2 = \mathrm{Tr}(H)/2$$

$$a_1 = \mathrm{Tr}(XH)/2$$

$$a_2 = \mathrm{Tr}(YH)/2$$

$$a_3 = \mathrm{Tr}(ZH)/2$$

Exercise: Suzuki-Trotter expansion

- Show that, given two non-commuting operators A, B with $[A, B] \neq 0$
$$e^{x(A+B)} = e^{xA}e^{xB} + O(x^2)$$

- Show that the decomposition $e^{x(A+B)} \approx e^{xB/2}e^{xA}e^{xB/2}$ provides a better approximation.

Hint: expand $e^{x(A+B)} = \mathbb{I} + x(A+B) + \frac{1}{2}x^2(A+B)^2 + O(x^3)$ *and compare it with the product of the separate expansions of* e^{xA} *and* e^{xB}

Remember this for quantum simulations https://arxiv.org/pdf/math-ph/0506007v1.pdf