Quantum Systems

(Lecture 2: The mathematical framework)

Luís Soares Barbosa

Universidade do Minho

Probabilistic states

- Classical bits are represented by Boolean values 0 and 1
- A probabilistic (classical) state can be represented by a vector of probabilities, e.g. the state 0 by a vector assigning probability 1 to 0 and 0 to 1, and similarly for state 1:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- If the state combines two probabilistic bits, say,

$$\begin{bmatrix} p_0 \\ p_1 \end{bmatrix} \qquad \begin{bmatrix} q_0 \\ q_1 \end{bmatrix}$$

it has 4 possibilities $\{00, 01, 10, 11\}$ each with a probability obtained by multiplying the corresponding probabilities of each component:

$$\begin{bmatrix} p_0 q_0 \\ p_0 q_1 \\ p_1 q_0 \\ p_1 q_1 \end{bmatrix} = \begin{bmatrix} p_0 \\ p_1 \end{bmatrix} \otimes \begin{bmatrix} q_0 \\ q_1 \end{bmatrix}$$

where $\otimes$ is the vectorial tensor product.

Quantum states

A quantum (binary) state is represented as a superposition, i.e. a linear combination of vectors $|0\rangle$ and $|1\rangle$ with complex coeficients:

$$|\phi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix}\alpha \\ \beta\end{bmatrix}$$

When state $|\phi\rangle$ is measured (i.e. observed) one of the two basic states $|0\rangle, |1\rangle$ is returned with probability

$$\| \alpha \|^2 \quad \text{and} \quad \| \beta \|^2$$

respectively.
Being probabilities, the norm squared of coefficients must satisfy

$$\| \alpha \|^2 + \| \beta \|^2 = 1$$

which enforces quantum states to be represented by unit vectors.

Vector spaces

Complex vector space

A set U of vectors generates a complex vector space whose elements can be written as linear combinations of vectors in U:

$$|v\rangle = a_1|u_1\rangle + a_2|u_2\rangle + \cdots + a_n|u_n\rangle$$

i.e.

- Abelian group $(V, +, -^1, 0)$
- with scalar multiplication $(c \cdot |v\rangle$ distributing over $+$, often represented by juxtaposition)

The Dirac notation

The symbol labelling a vector is written inside a

$$|\rangle$$

i.e. $|a\rangle$ rather than e.g. $\tilde{a}$

- Once a basis is chosen $|a\rangle$ can be represented as a column vector.
- Typically, the spaces of interest will have dimension 2^n, for an integer $n > 0$, because, as in the classical case, larger state spaces are obtained from smaller ones, usually of size 2.

The Dirac notation

In the computational basis — $\{|0\rangle, |1\rangle\}$ — the 2^n basis vectors are labelled by binary strings of length 2, e.g. for $n = 3$

$$|000\rangle = \begin{bmatrix}1\\0\\0\\0\\0\\0\\0\\0\end{bmatrix} \quad |001\rangle = \begin{bmatrix}0\\1\\0\\0\\0\\0\\0\\0\end{bmatrix} \quad \cdots \quad |110\rangle = \begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\0\end{bmatrix} \quad |111\rangle = \begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{bmatrix}$$

The Dirac notation

An arbitrary state is written as a superposition. For example, for $n = 3$, state

$$\sqrt{\frac{2}{3}}|01\rangle + \frac{i}{\sqrt{3}}|11\rangle \;=\; \sqrt{\frac{2}{3}}|0\rangle \otimes |1\rangle + \frac{i}{\sqrt{3}}|1\rangle \otimes |1\rangle$$

in Dirac notation corresponds to the column vector

$$\begin{bmatrix} 0 \\ \sqrt{\frac{2}{3}} \\ 0 \\ \frac{i}{\sqrt{3}} \end{bmatrix}$$

Note that

$$\left\|\frac{i}{\sqrt{3}}\right\|^2 + \left\|\sqrt{\frac{2}{3}}\right\|^2 = \left(\sqrt{\frac{i}{\sqrt{3}} x \frac{-i}{\sqrt{3}}}\right)^2 + \left(\sqrt{\sqrt{\frac{2}{3}} x \sqrt{\frac{2}{3}}}\right)^2 = 1$$

Hilbert spaces

Complex, inner-product vector space

A complex vector space with inner product

$$\langle - | - \rangle : V \times V \longrightarrow \mathbb{C}$$

such that

$$\begin{array}{ll} (1) & \langle v | \sum_i \lambda_i \cdot |w_i\rangle\rangle \;=\; \sum_i \lambda_i \langle v | w_i \rangle \\ (2) & \langle v | w \rangle = \overline{\langle w | v \rangle} \\ (3) & \langle v | v \rangle \geq 0 \;\; \text{(with equality iff } |v\rangle = 0\text{)} \end{array}$$

Note: $\langle - | - \rangle$ is conjugate linear in the first argument:

$$\langle \sum_i \lambda_i \cdot |w_i\rangle | v \rangle \;=\; \sum_i \overline{\lambda_i} \langle w_i | v \rangle$$

Notation: $\langle v | w \rangle \;\equiv\; \langle v, w \rangle \equiv (|v\rangle, |w\rangle)$

Hilbert spaces

Dot product

A useful example of a inner product is the dot product

$$\langle u|v\rangle = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} \cdot \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \underbrace{\begin{bmatrix} \overline{u_1} & \overline{u_2} & \cdots & \overline{u_n} \end{bmatrix}}_{\langle u|} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \sum_{i=1}^{n} \overline{u_i} v_i$$

where $\overline{c} = a - ib$ is the complex conjugate of $c = a + ib$

$\langle u|$ is the adjoint of vector $|u\rangle$, i.e a vector in the dual vector space $V^\dagger$.

Hilbert spaces

Dual space

If V is a Hilbert space, $V^\dagger$ is the space of linear maps from V to $\mathcal{C}$.

Elements of $V^\dagger$ are denoted by

$$\langle u| : V \longrightarrow \mathcal{C} \text{ defined by } \langle u|(|v\rangle) = \langle u|v\rangle$$

In a matricial representation $\langle u|$ is obtained as the Hermitian conjugate (i.e. the transpose of the vector composed by the complex conjugate of each element) of $|u\rangle$, therefore the dot product of $|u\rangle$ and $|v\rangle$.

Dirac's notation

Dirac's bra/ket notation is a handy way to represent elements and constructions on an Hilbert space, amenable to calculations and with direct correspondence to diagrammatic (categorial) representations of process theories

- $|u\rangle$ A ket stands for a vector in an Hilbert space V. In $\mathcal{C}^n$, a column vector of complex entries. The identity for $+$ (the zero vector) is just written 0.
- $\langle u|$ A bra is a vector in the dual space $V^\dagger$, i.e. scalar-valued linear maps in V — a row vector in $\mathcal{C}^n$.

There is a bijective correspondence between $|u\rangle$ and $\langle u|$

$$|u\rangle = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} \Leftrightarrow \begin{bmatrix} \overline{u}_1 \cdots \overline{u}_n \end{bmatrix} = \langle u|$$

A tradition going back to Penrose in the 1970's.

Bases

Old friends

- $|v\rangle$ and $|w\rangle$ are orthogonal if $\langle v|w\rangle = 0$
- norm: $\| \, |v\rangle \, \| = \sqrt{\langle v|v\rangle}$
- normalization: $\frac{|v\rangle}{\||v\rangle\|}$
- $|v\rangle$ is a unit vector if $\| \, |v\rangle \, \| = 1$
- A set of vectors $\{|i\rangle, |j\rangle, \cdots, \}$ is orthonormal if each $|i\rangle$ is a unit vector and

$$\langle i|j\rangle \;=\; \delta_{i,j} \;=\; \begin{cases} i = j & \Rightarrow 1 \\ \text{otherwise} & \Rightarrow 0 \end{cases}$$

Bases

Orthonormal basis

A orthonormal basis for a Hilbert space V of dimension 2^n is a set $B = \{|i\rangle\}$ of 2^n linearly independent elements of V st spanning V

- $\langle i|j\rangle = \delta_{i,j}$ for all $|i\rangle, |j\rangle \in B$
- and spans V, i.e. st every $|v\rangle$ in V can be written as

$$|v\rangle \ = \ \sum_i \alpha_i |i\rangle \quad \text{for some } \alpha_i \in \mathcal{C}$$

Note that the amplitude or coefficient of $|v\rangle$ wrt $|i\rangle$ satisfies

$$\alpha_i \ = \ \langle i|v\rangle$$

Why?

Bases

$\alpha_i = \langle i|v\rangle$ because

$$\begin{aligned}\langle i|v\rangle &= \langle i|\sum_j \alpha_j j\rangle \\ &= \sum_j \alpha_j \langle i|j\rangle \\ &= \sum_j \alpha_j \delta_{i,j} \\ &= \alpha_i\end{aligned}$$

Note

If $|v\rangle$ is expressed wrt any orthonormal basis $\{|i\rangle\}$, i.e. $|v\rangle = \sum_i \alpha_i |i\rangle$, then

$$\| \, |v\rangle \, \| = \sum_i \| \, \alpha_i \, \|^2$$

Example: The Hadamard basis

One of the infinitely many orthonormal bases for a space of dimension 2:

$$|+\rangle = |\nearrow\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$
$$|-\rangle = |\nwarrow\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$$

Check normality, e. g.

$$\langle +|-\rangle \;=\; \frac{1}{2}(\langle 0| + \langle 1|)(|0\rangle - |1\rangle) \;=\; \frac{1}{2}\begin{bmatrix}1\\1\end{bmatrix}\cdot\begin{bmatrix}1\\-1\end{bmatrix} \;=\; \frac{1}{2}\begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}1\\-1\end{bmatrix} \;=\; 0$$

Check orthogonality, e. g.

$$\|\,|+\rangle\,\| \;=\; \sqrt{\langle +|+\rangle} \;=\; \sqrt{\frac{1}{2}(\langle 0| + \langle 1|)(|0\rangle + |1\rangle)} \;=\; \sqrt{\frac{1}{2}\begin{bmatrix}1\\1\end{bmatrix}\cdot\begin{bmatrix}1\\1\end{bmatrix}} \;=\; 1$$

Bases

A basis for $V^\dagger$

If $\{|i\rangle\}$ is an orthonormal basis for V, then

$$\{\langle i|\}$$

is an orthonormal basis for $V^\dagger$

Example: Computing $\langle u|v\rangle$

Clearly, the inner product of two vectors over the same orthonormal basis boils down to vector multiplication:

$$\begin{aligned}
\langle u|v\rangle &= \langle \sum_i u_i \, |i\rangle | \sum_j v_j \, |j\rangle\rangle \\
&= \sum_{i,j} \overline{u_i} v_j \delta_{i,j} \\
&= \sum_i \overline{u_i} v_i \\
&= \begin{bmatrix} \overline{u_1} \cdots \overline{u_n} \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}
\end{aligned}$$

Example: Computing $\langle u|v\rangle$

$$|u\rangle = \sqrt{\frac{2}{3}}|01\rangle + \frac{i}{\sqrt{3}}|11\rangle = \begin{bmatrix} 0 \\ \sqrt{\frac{2}{3}} \\ 0 \\ \frac{i}{\sqrt{3}} \end{bmatrix} \text{ and } |v\rangle = \sqrt{\frac{1}{2}}|10\rangle + \sqrt{\frac{1}{2}}|11\rangle = \begin{bmatrix} 0 \\ 0 \\ \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{2}} \end{bmatrix}$$

In matricial representation

$$\begin{bmatrix} 0 & \sqrt{\frac{2}{3}} & 0 & \frac{-i}{\sqrt{3}} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{2}} \end{bmatrix} = 0 \times 0 + \sqrt{\frac{2}{3}} \times 0 + 0 \times \sqrt{\frac{1}{2}} + \frac{-i}{\sqrt{3}} \times \sqrt{\frac{1}{2}}$$

$$= \frac{-i}{\sqrt{6}}$$

Example: Computing $\langle u|v\rangle$

In Dirac notation

$$
\begin{aligned}
\langle u|v\rangle &= \left(\sqrt{\frac{2}{3}}\langle 01| + \frac{-i}{\sqrt{3}}\langle 11|\right)\left(\sqrt{\frac{1}{2}}|10\rangle + \sqrt{\frac{1}{2}}|11\rangle\right) \\
&= \sqrt{\frac{2}{3}}\sqrt{\frac{1}{2}}\underbrace{\langle 01|10\rangle}_{0} + \sqrt{\frac{2}{3}}\sqrt{\frac{1}{2}}\underbrace{\langle 01|11\rangle}_{0} + \frac{-i}{\sqrt{3}}\sqrt{\frac{1}{2}}\underbrace{\langle 01|10\rangle}_{0} + \frac{-i}{\sqrt{3}}\sqrt{\frac{1}{2}}\langle 11|11\rangle \\
&= \frac{-i}{\sqrt{6}}
\end{aligned}
$$

Hilbert spaces

The complete picture

Complete, complex, inner-product vector space, complete meaning that any Cauchy sequence

$$|v_1\rangle, |v_2\rangle, \cdots$$

converges

$$\forall_{\epsilon>0}\, \exists_N\, \forall_{m,n>0} \quad \| \, |v_m\rangle, |v_n\rangle \, \| \leq \epsilon$$

This completeness condition is trivial in finite dimensional vector spaces

Actions

- Operators (often called gates) are linear transformations
- Measurements (also called observations)

Matrices as linear maps

Any $m \times n$ matrix M can be seen as a linear operator mapping vectors in $\mathcal{C}^n$ to vectors in $\mathcal{C}^m$. Linearity means that

$$M\left(\sum_j \alpha_j \left|v_j\right\rangle\right) = \sum_j \alpha_j \, M \left|v_j\right\rangle$$

holds, where the action of M in a m-dimensional vector corresponds to multiplication.

Operating with qubits

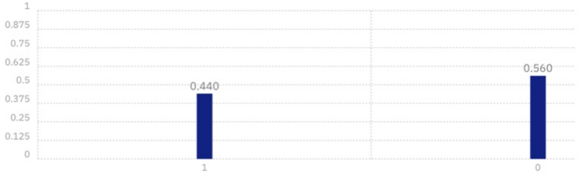
The $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ gate

$$X|0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

Operating with qubits

The H gate creates superpositions

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$



$$H|0\rangle = |+\rangle = \overbrace{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)}^{\text{superposition}}$$

$$H|1\rangle = |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Operating with qubits

Linear maps as matrices

Let V and W be vector spaces with basis, respectively,

$$B_V = \{|v_1\rangle, \cdots, |v_n\rangle\} \quad \text{and} \quad B_W = \{|w_1\rangle, \cdots, |w_m\rangle\}$$

A linear operator, i.e. a map $M : V \longrightarrow W$ st

$$M\left(\sum_j \alpha_j \,|v_j\rangle\right) = \sum_j \alpha_j \, M(|v_j\rangle)$$

can be represented by a $m \times n$ matrix st, for each $j \in 1..n$,

$$M(|v_j\rangle) = \sum_i M_{i,j} \,|w_i\rangle$$

Composition of linear operators amounts to multiplication of the corresponding matrices.
This representation is, of course, basis dependent.

Operators expressed in Dirac's notation

Dirac's notation provides a convenient way to specify linear transformations on quantum states:

outer product

$$|w\rangle\langle u|\,(|z\rangle) \;\widehat{=}\; |w\rangle\langle u||z\rangle \;=\; |w\rangle\,\langle u|z\rangle \;=\; \langle u|z\rangle\,|w\rangle$$

- matrix multiplication (composition of linear maps) is associative and scalars (zero objects in the corresponding universe) commute with everything

Operators expressed in Dirac's notation

In an orthonormal basis the operator

$$U = |i\rangle\langle j|$$

maps $|j\rangle$ to $|i\rangle$, because

$$U|j\rangle \; = \; |i\rangle \underbrace{\langle j||j\rangle}_{1} \; = \; |i\rangle$$

In the computational basis, $|i\rangle\langle j|$ is the matrix with 1 in position (i, j). Thus, the identity operator I can be written as

$$I \; = \; \sum_i |i\rangle\langle i|$$

Operators expressed in Dirac's notation

Example: $|0\rangle\langle 1|$

$$|0\rangle\langle 1| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

which has the following behaviour:
$|0\rangle\langle 1|$ maps $|1\rangle \mapsto |0\rangle$ and $|0\rangle \mapsto 0$

$$\begin{aligned} |0\rangle\langle 1|\,|1\rangle &= |0\rangle\,\langle 1|1\rangle = |0\rangle\,1 = |0\rangle \\ |0\rangle\langle 1|\,|0\rangle &= |0\rangle\,\langle 1|0\rangle = |0\rangle\,0 = 0 \end{aligned}$$

Operators expressed in Dirac's notation

Example: $X = |0\rangle\langle 1| + |1\rangle\langle 0|$

$$
\begin{aligned}
|0\rangle\langle 1| + |1\rangle\langle 0| \, (|0\rangle) &= |0\rangle\langle 1| \, (|0\rangle) + |1\rangle\langle 0| \, (|0\rangle) = 0 + |1\rangle = |1\rangle \\
|0\rangle\langle 1| + |1\rangle\langle 0| \, (|1\rangle) &= |0\rangle\langle 1| \, (|1\rangle) + |1\rangle\langle 0| \, (|1\rangle) = |0\rangle + 0 = |0\rangle
\end{aligned}
$$

represented by the following matrix in the computational basis:

$$
\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
$$

Operators expressed in Dirac's notation

Example: $|10\rangle\langle 00| + |00\rangle\langle 10| + |11\rangle\langle 11| + |01\rangle\langle 01|$

Maps $|00\rangle \mapsto |10\rangle$ and $|10\rangle \mapsto |00\rangle$
Clearly,

$$\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Operators expressed in Dirac's notation

A general operator A with entries a_{ij} in the standard basis can be written

$$A = \sum_i \sum_j a_{ij} |i\rangle\langle j|$$

Conversely, the i, j entry of the matrix for A in the standard basis is given by

$$\langle i|A|j\rangle$$

Why?

Operators expressed in Dirac's notation

$a_{ij} = \langle i|A|j\rangle$ because

$$\begin{aligned} A &= I\,A\,I \\ &= \sum_i |i\rangle\langle i|\; A \sum_j |j\rangle\langle j| \\ &= \sum_i \sum_j |i\rangle\langle i|A|j\rangle\langle j| \\ &= \sum_i \sum_j \underbrace{\langle i|A|j\rangle}_{a_{ij}} |i\rangle\langle j| \end{aligned}$$

Operators expressed in Dirac's notation

Example

Let $|s\rangle = \sum_k \beta_k |k\rangle$.

$$
\begin{aligned}
A|s\rangle &= \left(\sum_i \sum_j a_{ij}\,|i\rangle\langle j|\right) \left(\sum_k \beta_k |k\rangle\right) \\
&= \sum_i \sum_j \sum_k a_{ij}\,\beta_k\,|i\rangle\langle j|\,|k\rangle \\
&= \sum_i \sum_j a_{ij}\,\beta_j\,|i\rangle
\end{aligned}
$$

Operators expressed in Dirac's notation

In general, given a basis $B_V = \{|\beta_i\rangle\}$ for a N-dimensional Hilbert space V, an operator

$$A : V \longrightarrow V$$

can be written as

$$\sum_i \sum_j a_{ij} \, |\beta_i\rangle\langle\beta_j|$$

wrt this basis. The matrix entries are a_{ij}, as expected.

The Dirac's notation is

- independent of the basis and the order of the basis elements
- more compact
- and builds up intuitions ...