Quantum Computing (CST Part II)

Lecture 2: Linear Algebra

Quantum phenomena do not occur in a Hilbert space,
they occur in a laboratory.
Asher Peres

The need for linear algebra and Hilbert space

Quantum phenomena are described using linear algebra, which is the study of vector spaces and linear operations thereon. That is, states of a quantum system form a vector space and their transformations are described by linear operators.

A finite-dimension vector space with a defined *inner product* is also known as a **Hilbert space**, which is the most usual term used in the literature.

Recap: complex numbers and complex vectors

In general, we require complex numbers to describe quantum phenomena. Any $z \in \mathbb{C}$ is of the form $z = a + ib$ for some $a, b \in \mathbb{R}$ and $i = \sqrt{-1}$.

$\mathbb{C}^n$ is the vector space of n-tuples of complex numbers $\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}$.

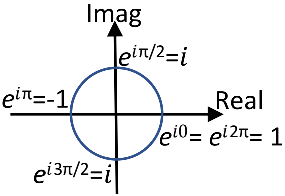
With addition: $\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} + \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} z_1 + w_1 \\ z_2 + w_2 \\ \vdots \\ z_n + w_n \end{bmatrix}$,

and scalar multiplication: $W \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} W z_1 \\ W z_2 \\ \vdots \\ W z_n \end{bmatrix}$.

More useful properties of complex numbers

Again letting $z = a + ib$ be a general complex number:

- Each complex number has a *conjugate*, $z^* = a - ib$
- The modulus of a complex number is given by $|z| = \sqrt{a^2 + b^2} = \sqrt{zz^*}$
- It can also be shown that for two complex numbers, z_1 and z_2, $|z_1 z_2| = |z_1||z_2|$.
- Unit complex numbers lie on the unit circle of the *Argand diagram*, and can be written in the form $e^{i\theta}$. θ is periodic with period 2π in the sense that $e^{i(\theta+2n\pi)} = e^{i\theta}$ for any $n \in \mathbb{Z}$.



Matrices

A matrix is an array of (in general) complex numbers:

$$A = \begin{bmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \\ a_{n1} & & a_{nm} \end{bmatrix}$$

With addition:

$$\begin{bmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \\ a_{n1} & & a_{nm} \end{bmatrix} + \begin{bmatrix} b_{11} & \dots & b_{1m} \\ \vdots & \ddots & \\ b_{n1} & & b_{nm} \end{bmatrix} = \begin{bmatrix} a_{11} + b_{11} & \dots & a_{1m} + b_{1m} \\ \vdots & \ddots & \\ a_{n1} + b_{n1} & & a_{nm} + b_{nm} \end{bmatrix}$$

and scalar multiplication:

$$B \begin{bmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \\ a_{n1} & & a_{nm} \end{bmatrix} = \begin{bmatrix} Ba_{11} & \dots & Ba_{1m} \\ \vdots & \ddots & \\ Ba_{n1} & & Ba_{nm} \end{bmatrix}$$

Matrix multiplication

If A is a $n \times m$ matrix and B is a $m \times l$ matrix then $C = A \times B$ is the $n \times l$ matrix with entries given by

$$C_{ik} = \sum_{j=1}^{m} A_{ij} B_{jk}$$

for all $i = 1, \ldots, n$ and $k = 1, \ldots, l$.

Matrix multiplication is

- Associative: $(A \times B) \times C = A \times (B \times C) = ABC$
- Distributive: $A(B + C) = AB + AC$; $(A + B)C = AC + BC$
- Not commutative: in general $AB \neq BA$. Note that BA won't even be mathematically meaningful unless $n = l$.

Tensor multiplication

As well as scalar multiplication and matrix multiplication, to describe quantum computation we must consider a third form of multiplication on matrices, *tensor multiplication*. Let A and B be matrices of any dimension:

$$A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1m}B \\ \vdots & \ddots & \\ a_{n1}B & & a_{nm}B \end{bmatrix}$$

where $\otimes$ denotes the tensor product. For example:

$$\begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \otimes \begin{bmatrix} 1 & 2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 4 & 6 \end{bmatrix}$$

In general if A is $n \times m$ and B is $n' \times m'$ then $A \otimes B$ is $nn' \times mm'$.

The tensor product is associative, so $A \otimes (B \otimes C) = (A \otimes B) \otimes C$.

Combining matrix and tensor multiplication

As a (column) vector is just a $n \times 1$ matrix, we can equally well apply tensor products to vectors. This reveals an important property of tensor products when combined with matrix products. Let A and B be $n \times m$ and $n' \times m'$ matrices respectively, and $\mathbf{x}$ and $\mathbf{y}$ be m and m' dimension column vectors respectively:

$$(A \otimes B)(\mathbf{x} \otimes \mathbf{y}) = (A\mathbf{x}) \otimes (B\mathbf{y})$$

The second exercise sheet asks you to prove this for the case of 2×2 matrices (note this separation also applies to matrices multiplying other matrices, i.e., if $\mathbf{x}$ and $\mathbf{y}$ were replaced by matrices of appropriate dimension).

Transpose and conjugate transpose (adjoint)

Let A be the $n \times m$ matrix:

$$A = \begin{bmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \\ a_{n1} & & a_{nm} \end{bmatrix}$$

A can be “transposed” by swapping its rows and columns. That is, the transpose of A is defined as the $m \times n$ matrix:

$$A^T = \begin{bmatrix} a_{11} & \dots & a_{n1} \\ \vdots & \ddots & \\ a_{1m} & & a_{mn} \end{bmatrix}$$

Slide 4 defined the conjugate of a complex number, $z = a + bi$, as $z^* = a - bi$. Combining this with the transpose, we get the *conjugate transpose* or adjoint of a matrix:

$$A^\dagger = (A^*)^T = \begin{bmatrix} a^*_{11} & \dots & a^*_{n1} \\ \vdots & \ddots & \\ a^*_{1m} & & a^*_{mn} \end{bmatrix}$$

It can be shown that $(AB)^T = B^T A^T$ and $(AB)^\dagger = B^\dagger A^\dagger$.

Dirac notation

Virtually all teaching and research on the subject of quantum information and computation expresses the linear algebra using *Dirac notation* (also known as “Bra-Ket” notation), and we will also adopt this convention.

By doing so, the expressions are compact, thus helping us to focus on the actual quantum states that are being represented.

“Bras” and “Kets”

A “Ket” is a column vector:

$$|\psi\rangle = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

Each “Ket” has a corresponding “Bra”, which is its conjugate transpose, the row vector:

$$\langle\psi| = \begin{bmatrix} a_1^* & a_2^* & \dots & a_n^* \end{bmatrix}$$

We continue to denote matrix operations with a capital letter, i.e., the matrix A operating on the state $|u\rangle$ would be written $A\,|u\rangle$.

When tensor multiplying vectors expressed as kets, the following are all equivalent: $|\psi\rangle \otimes |\phi\rangle$, $|\psi\rangle\,|\phi\rangle$, $|\psi\phi\rangle$ (and similarly for bras).

Also, as noted on Slide 7, tensor multiplication is associative, so $(|\psi\rangle \otimes |\phi\rangle) \otimes |\omega\rangle = |\psi\rangle \otimes (|\phi\rangle \otimes |\omega\rangle) = |\psi\phi\omega\rangle$ (again similarly for bras).

Inner products, orthogonality and norms

Let $|u\rangle = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}$, and $|v\rangle = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$, we define the inner product:

$$\langle u|v\rangle = \langle u| \times |v\rangle = \begin{bmatrix} a_1^* & \dots & a_n^* \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} = \sum_{i=1}^{n} a_i^* b_i$$

If each of $|u\rangle$ and $|v\rangle$ have at least one non-zero element:

- $\langle u|v\rangle = (\langle v|u\rangle)^*$
- If $\langle u|v\rangle = 0$ then $|u\rangle$ and $|v\rangle$ are orthogonal.
- $\langle u|u\rangle = \sum_{i=1}^{n} |a_i|^2$, which is a positive real number.
- $||\,|u\rangle\,|| = \sqrt{\langle u|u\rangle}$ is defined as the norm of $|u\rangle$, unit vectors have norm $= 1$.

Outer products and projectors

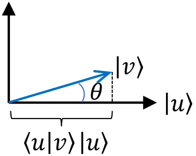
As well as inner products, vectors can be multiplied by outer-products, for which they need no longer have the same dimension. Let $|u\rangle = \begin{bmatrix} a_1 & \dots & a_n \end{bmatrix}^T$ and $|v\rangle = \begin{bmatrix} b_1 & \dots & b_m \end{bmatrix}^T$, the outer product is defined as the $n \times m$ complex matrix: $|u\rangle \langle v|$. That is:

$$|u\rangle \langle v| = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} \begin{bmatrix} b_1^* & \dots & b_m^* \end{bmatrix} = \begin{bmatrix} a_1 b_1^* & \dots & a_1 b_m^* \\ \vdots & \ddots & \\ a_n b_1^* & & a_n b_m^* \end{bmatrix}$$

If $|u\rangle$ is a unit vector, then $|u\rangle \langle u|$ is known as a *projector*, as $|u\rangle \langle u|$ is an operator that "projects" an arbitrary vector (of appropriate dimension) $|v\rangle$ onto the subspace $|u\rangle$. That is:

$$(|u\rangle \langle u|) |v\rangle = |u\rangle (\langle u| |v\rangle) = (\langle u|v\rangle) |u\rangle$$

which can be seen to be the projection of $|v\rangle$ onto $|u\rangle$:



Basis

A basis of $\mathbb{C}^n$ is a minimal collection of vectors $|v_1\rangle, |v_2\rangle, \dots, |v_n\rangle$ such that every vector $|v\rangle \in \mathbb{C}^n$ can be expressed as a linear combination of these:

$$|v\rangle = \alpha_1 |v_1\rangle + \alpha_2 |v_2\rangle + \cdots + \alpha_n |v_n\rangle$$

where the coefficients $\alpha_i \in \mathbb{C}$.

That the basis is a minimal collection of vectors means that $|v_1\rangle, |v_2\rangle, \dots, |v_n\rangle$ are linearly independent, no $|v_i\rangle$ can be expressed as a linear combination of the rest. The size of the basis is n, termed its *dimension*.

Of particular interest are *orthonormal bases*, in which each basis vector is a unit vector, and the basis vectors are pairwise orthogonal, that is:

$$\langle v_i | v_j \rangle = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Standard 'computational' basis

Here are some bases for $\mathbb{C}^3$:

$$\begin{bmatrix}1\\2\\1\end{bmatrix},\begin{bmatrix}10\\2+i\\0\end{bmatrix},\begin{bmatrix}1\\0\\0\end{bmatrix}\qquad\begin{bmatrix}0\\1/\sqrt{2}\\1/\sqrt{2}\end{bmatrix},\begin{bmatrix}0\\1/\sqrt{2}\\-1/\sqrt{2}\end{bmatrix},\begin{bmatrix}1\\0\\0\end{bmatrix}\qquad\begin{bmatrix}1\\0\\0\end{bmatrix},\begin{bmatrix}0\\1\\0\end{bmatrix},\begin{bmatrix}0\\0\\1\end{bmatrix}$$

The latter two of these are orthonormal, of which the final one is known as the standard or *computational* basis. In general, the computational basis for $\mathbb{C}^n$ is

$$|1\rangle=\begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix},|2\rangle=\begin{bmatrix}0\\1\\\vdots\\0\end{bmatrix},\ldots,|n\rangle=\begin{bmatrix}0\\0\\\vdots\\1\end{bmatrix}$$

Sometimes, especially in the case of two-level systems (i.e., for $\mathbb{C}^2$), we'll number these $|0\rangle\ldots|n-1\rangle$ (this will also apply to compositions of two-level systems).

Computational basis for compositions of two-level systems

Consider the computational basis for the composition of two two-level systems (we shall see that this corresponds to a two-qubit system). In this case, the basis is for $\mathbb{C}^4$, and has basis vectors:

$$
\begin{aligned}
|0\rangle = |00\rangle = |0\rangle \otimes |0\rangle &= \begin{bmatrix}1 & 0\end{bmatrix}^T \otimes \begin{bmatrix}1 & 0\end{bmatrix}^T = \begin{bmatrix}1 & 0 & 0 & 0\end{bmatrix}^T \\
|1\rangle = |01\rangle = |0\rangle \otimes |1\rangle &= \begin{bmatrix}1 & 0\end{bmatrix}^T \otimes \begin{bmatrix}0 & 1\end{bmatrix}^T = \begin{bmatrix}0 & 1 & 0 & 0\end{bmatrix}^T \\
|2\rangle = |10\rangle = |1\rangle \otimes |0\rangle &= \begin{bmatrix}0 & 1\end{bmatrix}^T \otimes \begin{bmatrix}1 & 0\end{bmatrix}^T = \begin{bmatrix}0 & 0 & 1 & 0\end{bmatrix}^T \\
|3\rangle = |11\rangle = |1\rangle \otimes |1\rangle &= \begin{bmatrix}0 & 1\end{bmatrix}^T \otimes \begin{bmatrix}0 & 1\end{bmatrix}^T = \begin{bmatrix}0 & 0 & 0 & 1\end{bmatrix}^T
\end{aligned}
$$

In general, if we have the composition of n two-level systems, then the computational basis is such that:

- When expressed as a ket, the number inside the ket is a n-bit binary number. Let this number be i.
- When expanded as a vector, we get a 2^n element vector, where each element is equal to zero, except for a single element equal to one, at the ith element (where the elements are indexed from 0 to $2^n - 1$).

It is really useful to remember this.

Expanding vectors and matrices in the standard basis

Any vector $|u\rangle = \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix}^T$ can be expressed as a weighted sum of standard basis vectors:

$$|u\rangle = a_1 |1\rangle + a_2 |2\rangle + \cdots + a_n |n\rangle$$

Similarly, any matrix can be expressed as a double sum over the outer-products of standard basis vectors:

$$\begin{bmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \\ a_{n1} & & a_{nm} \end{bmatrix} = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} |i\rangle \langle j|$$

Eigenvectors and eigenvalues

If a $n \times n$ matrix, A, has the effect of scaling a given (non-zero) vector, $|v\rangle$ by a constant, λ, then that vector is known as an *eigenvector*, with corresponding *eigenvalue* λ:

$$A\,|v\rangle = \lambda\,|v\rangle$$

The eigenvalues of a matrix are the roots of the characteristic polynomial:

$$\det(A - \lambda I) = 0$$

where $\det$ denotes the determinant, and I is the $n \times n$ identity. Each square matrix has at least one eigenvalue.

- The determinant of a matrix is the product of its eigenvalues.
- The trace of a square matrix is the sum of its leading diagonal elements. It is also the sum of its eigenvalues.

Diagonal representation of matrices

Recall from Slide 17 that any matrix can be expressed as a *double* sum, however some matrices can be expressed as a *single* sum. If a $n \times n$ complex matrix A can be expressed in the form:

$$A = \sum_{i=1}^{n} \lambda_i \left|v_i\right\rangle \left\langle v_i\right|$$

where λ_i is the ith eigenvalue of A, corresponding to the ith eigenvector, $\left|v_i\right\rangle$, then it is said to be diagonalisable. This is called the eigendecomposition, or spectral decomposition of A.

If A is diagonalisable as above, then its (normalised) eigenvectors form an orthonormal set, and A can be written as the diagonal matrix

$$\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

in the basis of its eigenvectors $\left|v_1\right\rangle$, $\left|v_2\right\rangle$, $\ldots$, $\left|v_n\right\rangle$. By this we mean that if an arbitrary vector, $\left|\psi\right\rangle$ is expressed as a weighted sum of the eigenvectors of A, i.e., $\left|\psi\right\rangle = a_1 \left|v_1\right\rangle + a_2 \left|v_2\right\rangle \ldots a_n \left|v_n\right\rangle$, then we would write $\left|\psi\right\rangle = \begin{bmatrix} a_1 & a_2 & \ldots a_n \end{bmatrix}$ “in the basis of its eigenvectors”.

Normal, Hermitian and unitary matrices

- A matrix is *normal* if $A^\dagger A = AA^\dagger$
  - A matrix is normal if and only if it is diagonalisable[1].
  - If $A = A^\dagger$ a matrix is *Hermitian*.
- A matrix is *unitary* if $A^\dagger A = AA^\dagger = I$ (the identity).
  - Unitary matrices play an important role in quantum computing.
  - Clearly all unitary matrices are normal therefore diagonalisable.
  - All eigenvalues of unitary matrices have absolute value one.
  - Unitary operators preserve inner products: if U is unitary and $|u'\rangle = U|u\rangle$ and $|v'\rangle = U|v\rangle$ then:

$$\begin{aligned}
\langle u'|v'\rangle &= (U|u\rangle)^\dagger(U|v\rangle) \\
&= (\langle u| U^\dagger)(U|v\rangle) \\
&= \langle u| (U^\dagger U) |v\rangle \\
&= \langle u| I |v\rangle \\
&= \langle u|v\rangle
\end{aligned}$$

[1] Note that the definition of “diagonalisable” that we have used in this lecture is the standard definition used in quantum mechanics, but elsewhere sometimes the slightly more general requirement that the eigenvectors form some (not necessarily orthonormal) basis is used.

Summary

We have covered a lot of ground in this lecture:

- Re-cap of the properties of complex vectors and matrices
- Tensor products
- Braket notation
- Inner products, orthogonality and norms
- Outer products and projectors
- Bases, the computational (standard) basis
- Eigenvectors, eigenvalues and diagonalisation
- Normal, Hermitian and unitary matrices