COL866: Quantum Computation and Information

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Quantum Mechanics: Linear Algebra

- Linear algebra: Study of vector spaces and linear operations on those vector spaces.
- The quantum mechanical notation of a vector in a vector space is $|\psi\rangle$, where ψ is the label for the vector.
- The zero vector of the vector space is denoted using $\mathbf{0}$. We do not use $|0\rangle$ since this is used to denote something else.
- A spanning set for a vector space is a set of vectors $|v_1\rangle, ..., |v_n\rangle$ such that any vector of the vector space can be written as a linear combination $|v\rangle = \sum_i a_i |v_i\rangle$.

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$$|v_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}; \quad |v_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

  - Question: Express $\left[\begin{smallmatrix} a_1 \\ a_2 \end{smallmatrix}\right]$ as a combination of $|v_1\rangle$ and $|v_2\rangle$.

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- A set of non-zero vectors is linearly dependent if there exists a set of complex numbers $a_1, ..., a_n$ with $a_i \neq 0$ for at least one value of i such that

$$a_1 |v_1\rangle + ... + a_n |v_n\rangle = \mathbf{0}$$

  A set of vectors is linearly independent if it is not linearly dependent.
  - Question: Are the vectors $\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 2 \\ 1 \end{bmatrix}$ linearly dependent?

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A set of vectors is linearly independent if it is not linearly dependent.
- Fact: Any two sets of linearly independent spanning sets contain the same number of vectors. Any such set is called a basis for the vector space. Moreover, such a basis set always exists.
- The number of elements in any basis is called the dimension of the vector space.
- In this course, we will only be interested in *finite dimensional* vector spaces.

- A linear operator between vector spaces V and W is defined to be any function $A : V \rightarrow W$ that is linear in its input:

$$A\left(\sum_i a_i |v_i\rangle\right) = \sum_i a_i A |v_i\rangle .$$

(We use $A|.\rangle$ in short to indicate $A(|.\rangle)$). A linear operator on a vector space V means that the linear operator is from V to V.

  - Example: Identity operator I_V on any vector space V satisfies $I_v |v\rangle = |v\rangle$ for all $|v\rangle \in V$.
  - Example: Zero operator 0 on any vector space V satisfies $0|v\rangle = \mathbf{0}$ for all $|v\rangle \in V$.
  - Claim: The action of a linear operator is completely determined by its action on the basis.

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- Composition: Given vector spaces V, W, X and linear operators $A : V \to W$ and $B : W \to X$, then BA denotes the linear operator from V to X that is a composition of operators B and A. We use $BA\left|v\right\rangle$ to denote $B(A(\left|v\right\rangle))$.

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- Matrix representation: Let $A : V \rightarrow W$ be a linear operator and let $\left|v_1\right\rangle, ..., \left|v_m\right\rangle$ be basis for V and $\left|w_1\right\rangle, ..., \left|w_n\right\rangle$ be basis for W. Then for every $1 \leq j \leq m$, there are complex numbers $A_{1j}, ..., A_{nj}$ such that

$$A\left|v_j\right\rangle = \sum_i A_{ij}\left|w_i\right\rangle.$$

  - Question: Let V be a vector space with basis $\left|0\right\rangle, \left|1\right\rangle$ and $A : V \rightarrow V$ be a linear operator such that $A\left|0\right\rangle = \left|1\right\rangle$ and $A\left|1\right\rangle = \left|0\right\rangle$. Give the matrix representation of A.

- Inner product: Inner product is a function that takes two vectors and produces a complex number (denoted by $(.,.)$).
- A function $(.,.)$ from $V \times V \rightarrow \mathbb{C}$ is an inner product if it satisfies the requirement that:
    1. $(.,.)$ is linear in the second argument. That is

$$\left(|v\rangle, \sum_i \lambda_i |w_i\rangle \right) = \sum_i \lambda_i (|v\rangle, |w_i\rangle).$$

    2. $(|v\rangle, |w\rangle) = (|w\rangle, |v\rangle)^*$.
    3. $(|v\rangle, |v\rangle) \geq 0$ with equality if and only if $|v\rangle = 0$.
- Question: Show that $(\sum_i \lambda_i |w_i\rangle, |v\rangle) = \sum_i \lambda_i^* (|w_i\rangle, |v\rangle)$.

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  3. $(|v\rangle, |v\rangle) \geq 0$ with equality if and only if $|v\rangle = 0$.
- Inner Product Space: A vector space equipped with an inner product is called an inner product space.
- In finite dimensions, a Hilbert space is simply an inner product space.

- Dual vector: $\langle v|$ is used to denote the dual vector to the vector $|v\rangle$. The dual is a linear operator from an inner product space V to complex number $\mathbb{C}$, defined by $\langle v|\left(|w\rangle\right) \equiv \langle v|w\rangle \equiv \left(|v\rangle, |w\rangle\right)$.
- Orthogonal: Vectors $|w\rangle$ and $|v\rangle$ are orthogonal if their inner product is 0.
- Norm: The norm of a vector $|v\rangle$ denoted by $||\,|v\rangle\,||$ is defined as:

$$||\,|v\rangle\,|| = \sqrt{\langle v|v\rangle}$$

- Unit vector: A unit vector is a vector $|v\rangle$ such that $||\,|v\rangle\,|| = 1$.
- Normalized vector: $\frac{|v\rangle}{|||v\rangle||}$ is called the normalized form of vector $|v\rangle$.
- Orthonormal set: A set of vectors $|1\rangle, ..., |n\rangle$ is orthonormal if each vector is a unit vector and distinct vectors in the set are orthogonal. That is $\langle i|j\rangle = \delta_{ij}$.

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- Let $|w_1\rangle, ..., |w_d\rangle$ be a basis set for some inner product space V. The following method, called the Gram-Schmidt procedure, produces an orthonormal basis set $|v_1\rangle, ..., |v_d\rangle$ for the vector space V.

Gram-Schmidt procedure

- $|v_1\rangle = \frac{|w_1\rangle}{|||w_1\rangle||}$.
- For $1 \leq k \leq d-1$, $|v_{k+1}\rangle$ is inductively defined as:

$$|v_{k+1}\rangle = \frac{|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i|w_{k+1}\rangle |v_i\rangle}{||\,|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i|w_{k+1}\rangle |v_i\rangle\,||}$$

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- Question Show that the Gram-Schmidt procedure produces an orthonormal basis for V.

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- Theorem: Any finite dimensional inner product space of dimension d has an orthonormal basis $|v_1\rangle, ..., |v_d\rangle$.

- Orthonormal set: A set of vectors $|1\rangle, ..., |n\rangle$ is orthonormal if each vector is a unit vector and distinct vectors in the set are orthogonal. That is $\langle i|j\rangle = \delta_{ij}$.
- Consider an orthonormal basis $|1\rangle, ..., |n\rangle$ for an inner product space V. Let $|v\rangle = \sum_i v_i |i\rangle$ and $|w\rangle = \sum_i w_i |i\rangle$. Then

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$$\langle v|w\rangle = \left(\sum_i v_i |i\rangle, \sum_j w_j |j\rangle\right) = \sum_{ij} v_i^* w_j \delta_{ij} = \begin{bmatrix} v_1^* & \dots & v_n^* \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_n \end{bmatrix}$$

- Dual vector $\langle v|$ has a row vector representation as seen above.

- Outer product: Let $|v\rangle$ be a vector in an inner product space V and $|w\rangle$ be a vector in the inner product space W. $|w\rangle\langle v|$ is a linear operator from V to W defined as:

$$(|w\rangle\langle v|)(|v'\rangle) \equiv |w\rangle\langle v|v'\rangle = \langle v|v'\rangle|w\rangle.$$

- $\sum_i a_i |w_i\rangle\langle v_i|$ is a linear operator which acts on $|v'\rangle$ to produce $\sum_i a_i |w_i\rangle\langle v_i|v'\rangle$.
- Completeness relation: Let $|i\rangle$'s denote orthonormal basis for an inner product space V. Then $\sum_i |i\rangle\langle i| = I$ (the identity operator on V).
- Claim: Let $|v_i\rangle$'s denote the orthonormal basis for V and $|w_j\rangle$'s denote orthonormal basis for W. Then any linear operator $A : V \to W$ can be expressed in the outer product form as:

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For any two vectors $|v\rangle, |w\rangle$, $|\langle v|w\rangle|^2 \leq \langle v|v\rangle\langle w|w\rangle$.

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- Eigenvector: A eigenvector of a linear operator A on a vector space is a non-zero vector $|v\rangle$ such that $A|v\rangle = v|v\rangle$, where v is a complex number known as the eigenvalue of A corresponding to the eigenvector $|v\rangle$.
- Characteristic function: This is defined to be $c(\lambda) \equiv det(A - \lambda I)$, where *det* denotes determinant for matrices.
  - Fact: The characteristic function depends only on the operator A and not the specific matrix representation for A.
  - Fact: The solution of the characteristic equation $c(\lambda) = 0$ are the eigenvalues of the operator.
  - Fact: Every operator has at least one eigenvalue.
- Eigenspace: The set of all eigenvectors that have eigenvalue v form the eigenspace corresponding to eigenvalue v. It is a vector subspace.
- Diagonal representation: The diagonal representation of an operator A on vector space V is given by $A = \sum_i \lambda_i |i\rangle \langle i|$, where the vectors $|i\rangle$ form an orthonormal set of eigenvectors for A with corresponding eigenvalue λ_i.
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- Degenerate: When an eigenspace has more than one dimension, it is called degenerate. Consider the eigenspace corresponding to eigenvalue 2 in the following example:

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- Adjoint or Hermitian conjugate: For any linear operator A on vector space V, there exists a unique linear operator $A^\dagger$ on V such that for all vectors $|v\rangle, |w\rangle \in V$:

$$(|v\rangle, A|w\rangle) = (A^\dagger |v\rangle, |w\rangle)$$

Such a linear operator $A^\dagger$ is called the adjoint or Hermitian conjugate of A.

  - Exercise: Show that $(AB)^\dagger = B^\dagger A^\dagger$.
  - By convention, we define $|v\rangle^\dagger \equiv \langle v|$.
  - Exercise: Show that $(A|v\rangle)^\dagger = \langle v| A^\dagger$.
  - Exercise: Show that $(|w\rangle\langle v|)^\dagger = |v\rangle\langle w|$.
  - Exercise: $(\sum_i a_i A_i)^\dagger = \sum_i a_i^* A_i^\dagger$.
  - Exercise: Show that $(A^\dagger)^\dagger = A$.
  - Exercise: Show that in matrix representation, $A^\dagger = (A^*)^T$.

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- Hermitian or self-adjoint: An operator A with $A^\dagger = A$ is called Hermitian or self-adjoint.
- Projectors: Let W be a k-dimensional vector subspace of a d-dimensional vector space V. There is an orthonormal basis $|1\rangle, ..., |d\rangle$ for V such that $|1\rangle, ..., |k\rangle$ is an orthonormal basis for W. The projector onto the subspace W is defined as:

$$P \equiv \sum_{i=1}^{k} |i\rangle \langle i|$$

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  - Observation: The definition is independent of the orthonormal basis used for W.
  - Exercise: Projector P is Hermitian. That is $P^\dagger = P$.
  - Notation: We use vector space P as a shorthand for the vector space onto which P is a projector.
  - Exercise: Show that for any projector $P^2 = P$.
- Orthogonal complement: The orthogonal complement of a projector P is the operator $Q \equiv I - P$.
  - Exercise: Q is a projector onto the vector space spanned by $|k+1\rangle, ..., |d\rangle$.

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- Normal operator: An operator A is said to be normal if $AA^\dagger = A^\dagger A$.

Spectral Decomposition Theorem

Any normal operator M on a vector space V is a diagonalizable with respect to some orthonormal basis for V. Conversely, any diagonalizable operator is normal.

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- Exercise: Show that a normal matrix is Hermitian if and only if it has real eigenvalues.
- Unitary matrix: A matrix U is called unitary if $UU^\dagger = U^\dagger U = I$.
- Unitary operator: An operator U is unitary if $UU^\dagger = U^\dagger U = I$.
- Exercise: Show that unitary operators preserve inner products.
- Exercise: Let $|v_i\rangle$ be any orthonormal basis set and let $|w_i\rangle = U|v_i\rangle$. Then $|w_i\rangle$ is an orthonormal basis set. Moreover, $U = \sum_i |w_i\rangle\langle v_i|$.
- Exercise: If $|v_i\rangle$ and $|w_i\rangle$ are two orthonormal basis sets, then $U \equiv \sum_i |w_i\rangle\langle v_i|$ is a unitary operator.
- Exercise: Show that all the eigenvalues of a unitary matrix have modulus 1. This means that they can be written as $e^{i\theta}$ for some real θ.

- Positive operator: An operator A is said to be a positive operator if for every vector $|v\rangle$, $(|v\rangle, A|v\rangle)$ is a real non-negative number.
- Positive definite operator: An operator A is said to be a positive operator if for every vector $|v\rangle$, $(|v\rangle, A|v\rangle)$ is a real number strictly greater than 0.

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- Exercises:
  - Show that a positive operator is necessarily Hermitian.
  - Show that the eigenvectors of a Hermitian operator with different eigenvalues are necessarily orthogonal.
  - Show that for any operator A, $A^\dagger A$ is positive.
  - Show that the eigenvalues of a projector P are all either 0 or 1.

- The tensor product is a way of putting vector spaces together to form larger vector spaces.
  - Suppose V and W are Hilbert spaces of dimension m and n respectively, then $V \otimes W$ denotes an mn-dimensional vector space.
  - The elements of $V \otimes W$ are linear combinations of tensor products $|v\rangle \otimes |w\rangle$ of elements $|v\rangle \in V$ and $|w\rangle \in W$.
  - If $|i\rangle$'s and $|j\rangle$'s are orthonormal bases for V and W respectively, then $|i\rangle \otimes |j\rangle$'s are orthonormal basis for $V \otimes W$.
  - $|v\rangle \otimes |w\rangle$ is also written as $|vw\rangle$, $|v\rangle |w\rangle$, and $|v, w\rangle$.
  - Example: If V is a two-dimensional vector space with basis $\{|0\rangle, |1\rangle\}$, then $|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle$ is an element of $V \otimes V$.
- Notation: $|\psi\rangle^{\otimes k}$ means $|\psi\rangle$ tensored with itself k times.

- Some properties of tensor products:
  - For any arbitrary scalar z and elements $|v\rangle \in V$ and $|w\rangle \in W$:

$$z(|v\rangle \otimes |w\rangle) = (z\,|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z\,|w\rangle).$$

  - For arbitrary $|v_1\rangle, |v_2\rangle \in V$ and $|w\rangle \in W$,

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle.$$

  - For arbitrary $|v\rangle \in V$ and $|w_1\rangle, |w_2\rangle \in W$,

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle.$$

- Linear operators on $V \otimes W$: Let A and B be linear operators on V and W respectively. Then $A \otimes B$ denotes a linear operator on $V \otimes W$ defined as:

$$(A \otimes B)(|v\rangle \otimes |w\rangle) = A|v\rangle \otimes B|w\rangle .$$

Furthermore, the following ensures linearity:

$$(A \otimes B)\left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle\right) = \sum_i a_i A|v_i\rangle \otimes B|w_i\rangle .$$

- Let $A : V \to V'$ and $B : W \to W'$ be linear operators. An arbitrary linear operator C mapping $V \otimes W$ to $V' \otimes W'$ can be represented as a linear combination:

$$C = \sum_i c_i A_i \otimes B_i$$

where by definition:

$$\left(\sum_i c_i A_i \otimes B_i\right)|v\rangle \otimes |w\rangle \equiv \sum_i c_i A_i|v\rangle \otimes B_i|w\rangle .$$

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  $(\sum_i c_i A_i \otimes B_i)\,|v\rangle \otimes |w\rangle \equiv \sum_i c_i A_i\,|v\rangle \otimes B_i\,|w\rangle$.
- The inner product on $V \otimes W$ is defined as:

$$\left(\sum_i a_i\,|v_i\rangle \otimes |w_i\rangle\,, \sum_j b_j\,|v'_j\rangle \otimes |w'_j\rangle\right) \equiv \sum_{ij} a_i^* b_j \,\langle v_i|v'_j\rangle\,\langle w_j|w'_j\rangle\,.$$

Quantum Mechanics

Linear algebra: Tensor products

- Matrix representation: The matrix representation for $A \otimes B$ is called the Kronecker product. Let A be a $m \times n$ matrix and B be a $p \times q$ matrix. Then the matrix representation of $A \otimes B$ is given as:

$$A \otimes B \equiv \begin{bmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21} & A_{22}B & \dots & A_{2n}B \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{bmatrix}$$

  - Example: What is $\begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 2 \\ 3 \end{bmatrix}$?

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  - Example: What is $\begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 2 \\ 3 \end{bmatrix}$? $\begin{bmatrix} 2 \\ 3 \\ 4 \\ 6 \end{bmatrix}$

- Exercises:
  - Show that $(A \otimes B)^* = A^* \otimes B^*; (A \otimes B)^T = A^T \otimes B^T; (A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$.
  - Show that the tensor product of two unitary operators is unitary.
  - Show that the tensor product of two Hermitian operators is Hermitian.
  - Show that the tensor product of two positive operators is postive.
  - Show that the tensor product of two projectors is a projector.

- One can define matrix functions on normal matrices by using the following construction: Let $A = \sum_a a \left|a\right\rangle \left\langle a\right|$ be a spectral decomposition for a normal operator A. We define:

$$f(A) = \sum_a f(a) \left|a\right\rangle \left\langle a\right|$$

  - Exercise: Show that $exp(\theta Z) = \begin{bmatrix} e^{\theta} & 0 \\ 0 & e^{-\theta} \end{bmatrix}$.
  - Exercise: Find the square root of the matrix $\begin{bmatrix} 4 & 3 \\ 3 & 4 \end{bmatrix}$.

End