

Properties of Linear Algebra Applicable to Quantum Computing

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OUTLINE:

Mathematics and Physics Concepts Required to Describe a Quantum Computing System

- Introduce relevant mathematics applicable to quantum computing
- Introduce quantum mechanics axioms that describe observed physics
- Combine relevant mathematics with the physics of quantum mechanics to allow one to formulate
 - Design programming primitives that can aggregate into quantum computing algorithms
 - Program algorithms for implementation on quantum simulators and HW platforms
 - Configure and run these algorithms on quantum computing simulators and quantum computing hardware platforms

Theory of Quantum Mechanics Describes Behavior Observed in a Non-classical World

- In order to properly design quantum computing algorithms programs and physical devices to performs calculations based on the observables axioms of quantum mechanics one must
 - Understand the quantum mechanical properties and measured observables
 - Use appropriate mathematics to properly describes these properties and observables
- Quantum theory is a mathematical model of the physical world at a scale where the size of the observation being made are of the same order of magnitude as the size of the object being observed
 - Measuring the speed of a car moving on a road (classical)
 - Measuring the bound state energy of an electron in a hydrogen atom (quantum mechanical)
- Many of the observed behaviors of the physical world at the quantum level have no analogs in people's everyday (classical) experiences

Building a Rigorous Mathematical Foundation for Describing Quantum Computing

Utilize the Mathematics of Linear Algebra to Represent Quantum Computing Processes

Mathematics Applicable to Quantum Computing

- The axioms of quantum mechanics are well described by the mathematics of linear algebra
- Linear algebra concepts for describing a quantum computing system
 - Any given system is identified with some finite- or infinite-dimensional Hilbert space
 - The system can be mathematically represented as states
 - Pure states correspond to vectors of norm 1
 - This norm 1 set of all pure states can be graphically represented/visualized by a unit sphere in a Hilbert space

Review Basic Linear Algebra Concepts

- **Vector Space**: A vector space is a collection vectors, which may be added together and multiplied by scalar quantities and still be a part of that same collection of vectors
- The **adjoint** $\mathbf{a}^\dagger$ is the complex conjugate transpose of a column vector “ $\mathbf{a}$ ” and is sometimes called the Hermitian conjugate
- The space is complete as expressed by the norm

$$||\mathbf{a}|| = (\langle \mathbf{a} | \mathbf{a} \rangle)^{1/2}$$

Review Basic Linear Algebra Concepts

Linear Dependence and Linear Independence

- A set of vectors is said to be linearly dependent if one of the vectors in the set can be defined as a linear combination of the others
- A set of vectors is said to be linearly independent if no vector in the set can be written according to the previous statement

Review Basic Linear Algebra Concepts

Basis Vectors

A set of elements (vectors) in a vector space V is called a basis, or a set of basis vectors, if the vectors are

- linearly independent
- every vector in the vector space is a linear combination of this set

A basis is a linearly independent spanning set

Review Basic Linear Algebra Concepts

Properties and Definitions of a Vector Space

- Given a vector space V containing vectors A, B, C the following properties apply
 - Commutativity [$A+B=B+A$]
 - Associativity of vector addition [$(A+B)+C=A+(B+C)$]
 - Additive identity [$0+A=A+0=A$] for all A
 - Existence of additive inverse: For any A , there exists a $(-A)$ such that $A+(-A)=0$

Review Basic Linear Algebra Concepts

Properties and Definitions of a Vector Space

- Given a vector space V containing vectors A, B, C the following properties apply
 - Scalar multiplication identity [$1 \cdot A = A$]
 - Given scalars r and s
 - Associativity of scalar multiplication [$r(sA) = (rs)A$]
 - Distributivity of scalar sums [$(r+s)A = rA + sA$]
 - Distributivity of vector sums [$r(A+B) = rA + rB$]

Hilbert Space

- **Hilbert Space:** A Hilbert space is a vector space G that has an inner product $\langle \mathbf{u}, \mathbf{v} \rangle$ such that a norm

$$|\mathbf{u}| = \sqrt{\langle \mathbf{u}, \mathbf{u} \rangle}$$

turns G into a complete metric space. (A complete metric space is a metric space in which every Cauchy sequence is convergent)

- A Hilbert Space with vectors $\mathbf{a}$ and $\mathbf{b}$ may be defined over either the real or complex numbers with an inner product $\langle \mathbf{b} | \mathbf{a} \rangle$
- A Hilbert Space maps an ordered pair of vectors to the complex numbers with the following properties
 - Positivity $\langle \mathbf{a} | \mathbf{a} \rangle$ is greater than 0 for $|\mathbf{a} \rangle$ greater than 0
 - Linearity $\langle \mathbf{c} | (\alpha |\mathbf{a} \rangle + \beta |\mathbf{b} \rangle) = \alpha \langle \mathbf{c} | \mathbf{a} \rangle + \beta \langle \mathbf{c} | \mathbf{b} \rangle$ where α and β are complex constants
 - Skew symmetry $\langle \mathbf{b} | \mathbf{a} \rangle = (\langle \mathbf{a} | \mathbf{b} \rangle)^*$
- An example of a finite-dimensional Hilbert space is an n -dimensional vector space of the complex numbers $\mathbb{C}^n$ with $\langle \mathbf{u}, \mathbf{v} \rangle$ as the vector dot product of $\mathbf{u}$ and $\mathbf{v}^*$ (complex conjugate)

Dirac “bra” and “ket” Notation

Dirac “ket” notation $|a\rangle$ represents a column vector $\vec{a}$

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

a Dirac “bra” notation $\langle a|$

$$\langle a| = (a_1^* \quad a_2^* \quad \dots \quad a_n^*)$$

The transpose $\mathbf{a}^T$ of a column vector $\mathbf{a}$ is a row vector

Examples of Normalized Vectors in Dirac Notation

$$|a\rangle = \frac{1}{\sqrt{2}} [|0\rangle + |1\rangle] = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$|b\rangle = \left[\frac{3}{5}|0\rangle - \frac{4}{5}|1\rangle \right] = \frac{3}{5} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{4}{5} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{3}{5} \\ -\frac{4}{5} \end{pmatrix}$$

$$|c\rangle = \frac{3i}{5}|0\rangle - \frac{4i}{5}|1\rangle = \frac{3i}{5} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{4i}{5} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{3i}{5} \\ -\frac{4i}{5} \end{pmatrix}$$

Mathematical Representation of Binary States and Superposition

- A binary state (classical bit) defines a state by
- values of either “0” or “1” (“on” or “off”)



Mathematical Representation of Bits, Qubits and Superposition

- A classical bit defines a state by values of either “0” or “1” (“on” or “off”)
- A quantum bit (qubit) can also have a state of “0” or “1” but it can also have a possibility of being described by additional states



Mathematical Representation of Bits, Qubits and Superposition

- A classical bit defines a state by values of either “0” or “1” (“on” or “off”)
- A quantum bit (qubit) can also have a state of “0” or “1” and it can also have a possibility of being described by additional states
- Qubit can form a superposition state represented by a vector that is a superposition or linear combination of both a “0” or “1”

$$|a\rangle = \alpha|0\rangle + \beta|1\rangle \quad |\alpha|^2 + |\beta|^2 = 1$$



A Qubit

- A qubit is a quantum system described by a two-dimensional Hilbert space, whose state can take any value of the form

$$|a\rangle = \alpha|0\rangle + \beta|1\rangle$$

- We can perform a measurement that projects the qubit onto the basis $\{|0\rangle, |1\rangle\}$ which will measure an outcome of $|0\rangle$ with probability $|\alpha|^2$ and an outcome of $|1\rangle$ with probability $|\beta|^2$

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

- Qubit can form a superposition state represented by a vector that is a superposition or linear combination of both a “0” or “1”
- The coefficients α and β also encode the relative phase that has physical significance

Basis Vectors for One Qubit

- In Dirac notation a qubit can be represented by

$$a = \alpha|0\rangle + \beta|1\rangle \quad |\alpha|^2 + |\beta|^2 = 1 \text{ (modulus)}$$

where α and β are complex coefficients

- α is the probability amplitude of measuring the $|0\rangle$ state and β is the probability amplitude of measuring the $|1\rangle$ state
- Common basis is $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
- Probability to measure the $|0\rangle$ state is $|\alpha|^2$
- Probability to measure the $|1\rangle$ state is $|\beta|^2$
- Calculate $\langle 0|0\rangle$ and $\langle 1|1\rangle$ (gives an answer of a single number)

Constructing Matrices from Bras and Kets

If the bra and ket are placed in the opposite order

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

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

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

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

Outer products are a useful mechanism for writing matrices, especially unitaries because they capture state transformations

A Qubit

- Interpret a qubit from a geometric standpoint
- A $|0\rangle$ and $|1\rangle$ can represent opposite orientations of a vector in a three-dimensional space along a constructed set of axes in a coordinate system (example: z-axis with polar angle θ and azimuthal angle ϕ)
- A vector in this geometric construction can be transformed by rotations that express symmetries of the operations

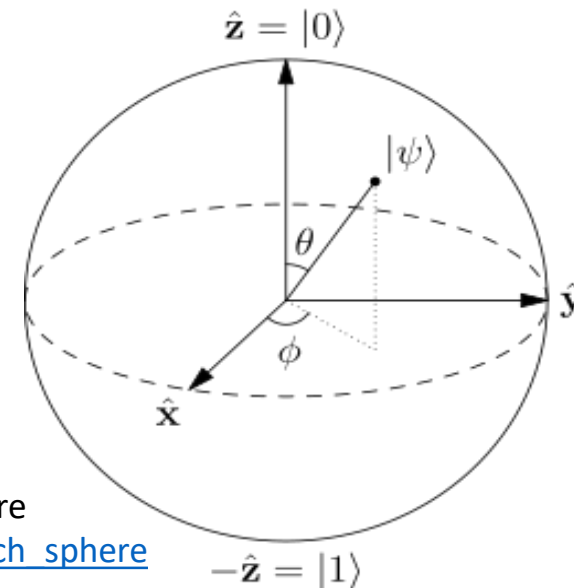


Figure from Wikipedia Bloch Sphere
https://en.wikipedia.org/wiki/Bloch_sphere

Symmetries and Spatial Rotations

- Consider the case of a three dimensional rotation
- Given a vector $\mathbf{v}$ one can perform an infinitesimal rotation of $\mathbf{v}$ by $d\Theta$ about the axis specified by a unit vector
- Mathematically $R(\hat{n}, d\Theta) = I - id\Theta \hat{n} \cdot \vec{J}$ where $\hat{n} = (n_1, n_2, n_3)$ are the components of angular rotations $\vec{J}$
- Basic properties of rotations can be written as commutation relations

$$[J_i, J_j] = J_i J_j - J_j J_i$$

$$[J_i, J_j] = i\epsilon_{ijk} J_k$$

where ϵ_{ijk} is the totally antisymmetric tensor and repeated indices are summed

Rotation Group

- Although the “defining” representation of the rotation group is three dimensional, the simplest nontrivial irreducible representation is two dimensional
- In this case there is a unique two-dimensional irreducible representation, up to a unitary change of basis.
- The generators of this rotation group are

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x$$

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z$$

Properties of These Rotation Matrices

- Matrices are mutually anticommuting
- They mathematically can be squared to the identity

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij}I \quad (\hat{n} \cdot \vec{\sigma})^2 = n_i n_j \sigma_i \sigma_j = n_i n_j I$$

- In spherical coordinates the pure density matrix can now be written

$$\rho(\hat{n}) = \frac{1}{2}(I + \hat{n} \cdot \vec{\sigma})$$

$$U(\hat{n}, \theta) = \exp(i \frac{\theta}{2} \hat{n} \cdot \vec{\sigma}) = I \cos(\frac{\theta}{2}) - i \hat{n} \cdot \vec{\sigma} \sin(\frac{\theta}{2})$$

Rotation Operators

- Write the exponential in terms of a series expansion

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k$$

- This gives rise to 3 useful classes of unitary matrices (rotation operators) when they are exponentiated

$$e^{-i\sigma \cdot \hat{n} \frac{\theta}{2}} = \cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right) \sigma \cdot \hat{n}$$

$$R_{\hat{n}}(\theta) \equiv e^{-i\theta \hat{n} \cdot \frac{\sigma}{2}} = \cos\left(\frac{\theta}{2}\right) I - i\sin\left(\frac{\theta}{2}\right) (n_x X + n_y Y + n_z Z)$$

Rotation Group

- The “defining” representation of the rotation group is three dimensional, but the simplest nontrivial irreducible representation is two dimensional
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Pauli X — X — $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x$

Pauli Y — Y — $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y$

Pauli Z — Z — $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z$

Pauli Spin Matrices*

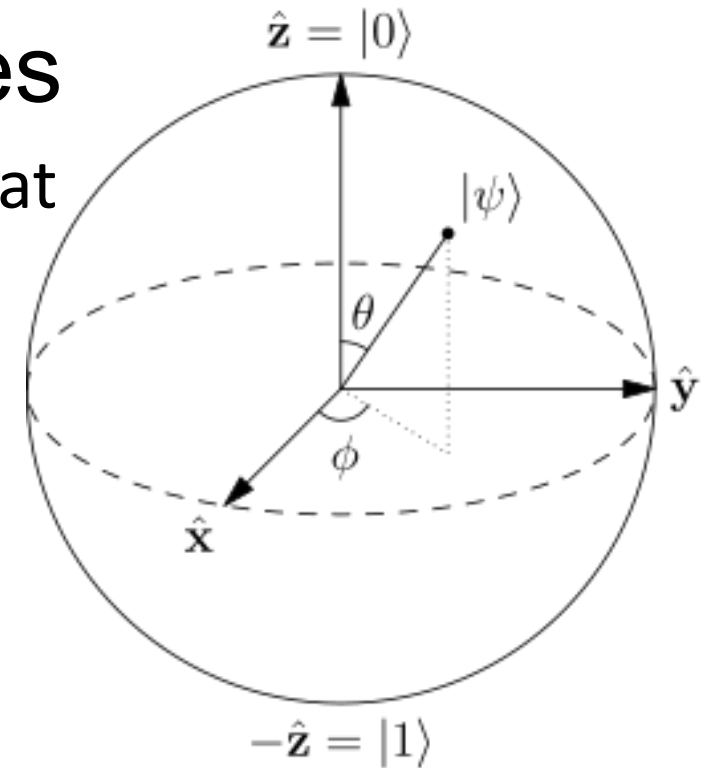
* These Pauli Spin Matrices have a special relationship in physics to particles that carry a property known as “spin”

Mathematical Representation of Many Different Basis States

- Represent combination of “0”s and “1”s in a way that many different values can be expressed
- Define $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
- Can re-write $|a\rangle = \alpha|0\rangle + \beta|1\rangle$ as $|\alpha|^2 + |\beta|^2 = 1$

$$|a\rangle = e^{i\gamma} \left(\cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle \right)$$

- This representation is visualized by states that lie on the surface of a Bloch sphere
- The Bloch sphere is a geometrical representation of the pure state space of a two-level quantum mechanical system



Bloch Sphere

Figure from Wikipedia Bloch Sphere
https://en.wikipedia.org/wiki/Bloch_sphere

Matrices as Rotations Acting on Qubits

- Matrices describe the rotations that takes a qubit from an initial state to a transformed state
- These rotations that operate on a qubit are labelled as “gates”
- Because qubit states can be represented as points on a sphere, reversible one-qubit gates can be thought of as rotations of the Bloch sphere. (quantum gates are often called “rotations”)
- Reversible one qubit gates viewed as rotations in this three dimensional representation

Construct Rotation Matrices From Bra and Ket Vectors

- The matrix representation of the expression $\sum_i |input_i\rangle\langle output_i|$

$$I = |0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$X = |0\rangle\langle 1| + |1\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

$$H = \frac{1}{\sqrt{2}} [(|0\rangle + |1\rangle)\langle 0| + (|0\rangle - |1\rangle)\langle 1|] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Questions