Generating images with a quantum computer

BATXILLERAT'S RESEARCH WORK IES MIQUEL TARRADELL

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Chapter 1

Introduction

Desde hace más de un año, me he dedicado a estudiar computación cuántica durante mi tiempo libre. Buscaba investigar un campo relacionado con la mecánica cuántica, pero sin que sea muy complicado, que se pueda entender a un nivel teórico y que me entusiasme.

La Computación Cuántica (concretamente Teoría de la Información Cuántica) encaja perfectamente con esos criterios. Es más sencilla que la mecánica cuántica debido a que no está basada en cálculo o ecuaciones diferenciales, se basa en la álgebra lineal. Siempre se emplean valores discretos, vectores y matrices. Además si se trabaja a un nivel teórico sencillo no se tienen en consideración las interpretaciones físicas, lo cual simplifica mucho las cosas. Cuanto más me adentraba, más ganas tenía de seguir.

Mi parte favorita de este campo es el Quantum Machine Learning que consiste en diseñar y aplicar conceptos de Machine Learning a los ordenadores cuánticos, como por ejemplo implementar cuánticamente las famosas Redes Neuronales, que estan detrás de la mayoria de inteligencias artificiales que vemos hoy en día.

QML es un campo de investigación joven y en crecimiento debido a que sus algoritmos son ideales para implementarlos con los ordenadores cuánticos actuales, los cuales no son muy potentes. Ejemplos de estas implementaciones serían algoritmos de generación y clasificación de dígitos, clasificación de datos no etiquetados, control de operaciones cuánticas, análisis de datos de aceleradores de partículas, etc.

De entre todos los tipos de algoritmos me he centrado en las Redes Neuronales Cuánticas, análogas cuánticas de las Redes Neuronales tan utilizadas hoy en día para hacer gran variedad de tareas. Me he interesado particularmente en ellas debido a que tenía experiencia en el pasado con las RR clásicas y había visto que existen frameworks de software para trabajar con ellas como TensorFlow Quantum que me podían ayudar.

Para adentrarme en el campo de QML, he tenido que adquirir conocimientos en álgebra lineal, cálculo y física. Dentro de QML en concreto me he dedicado a leer papers que me interesan y en un par de ocasiones intentar implementar los algoritmos detallados en esos papers. Puede parecer algo imposible en principio debido a que no tengo acceso directo a un ordenador cuántico, no obstante estos no son necesarios debido a que las operaciones cuánticas pueden ser simuladas en un ordenador corriente de escritorio (con ciertas limitaciones). Pero en reaque puedo tener acceso a ordenadores cuánticos ya que IBM permite acceder a los suyos mediante IBM Quantum Experience, aunque nunca he dado uso de ello debido a que no lo veía necesario.

En este trabajo de investigación me he propuesto implementar mediante código uno de los algoritmos que he visto en un paper, una Red Adversaria Generativa Cuàntica (GAN, en inglés) que genera dígitos binarios (unos y ceros) a partir de un circuito cuántico. Como objetivo tengo verificar una sugerencia que hacen los autores del paper: implementar una función no-lineal en una parte del algoritmo que podría mejorar el rendimiento de este. Mi hipótesis al igual que los autores (aunque ellos lo comentan muy brevemente) es que el algoritmo va a reducir ligeramente el número de interacciones que son necesarias para llegar a su punto óptimo. Es decir, el modelo con la función no-lineal va a necesitar menos operaciones que lo entren conseguir los mismos resultados que el modelo sin la función.

Chapter 2

Theoretical Framework

2.1 Linear Algebra

When I start looking into quantum computation, I realized quickly that I needed more mathematical knowledge to understand the mathematical notation and concepts that were on the QC textbooks. By that time I came across the wonderful video lectures on lineal algebra -which is the branch of mathematics that is the background for QC- by Prof. Gilbert Strang at MIT. I watched nearly all of them along a part of the complementary videos that went through the homework.

Those lectures really helped me to understand the math on [citation] and [citation]. And little by little I learned the math notation used in quantum mechanics, the Dirac notation.

In the current section I will be going through the basic concepts of linear algebra, to form the mathematical background used along this work.

2.1.1 Vectors and Vector Spaces

The basic objects of linear algebra are vector spaces. A vector space is the set of all the vectors that have the same dimensions. For example \mathbb{R}^3 would be the vector space of all 3 dimensional vectors that can be used to represent all possible coordinates on a 3D space. In QC and QI a special kind of vector spaces are used: Hilbert spaces, in other words, an inner product space. Hilbert

spaces follow a set of products and have certain properties, on section 2.1 I'll be going through a part of those products and properties, the amount that is compulsory. Keep in mind that Hilbert spaces are much more complicated than what is presented here. Keep in mind that when mentioning a vector space in this work, that vector space is a complex Hilbert space, unless it's specified otherwise.

Vector spaces are defined by their bases, a set of vectors $B = \{|v_1\rangle, \dots, |v_n\rangle\}$ is a valid base for a vector space V if any vector $|v\rangle$ in it, can be written as $|v\rangle = \sum_i a_i \, |v_i\rangle$ for $|v_i\rangle \in B$. Every vector in B are linearly independent to each other.

The standard notation for linear algebra concepts in quantum mechanics is the Dirac notation, which represents a vector as $|\psi\rangle$. Where ψ is the label of the vector. A vector $|\psi\rangle$ with n dimensions can be also represented as a column matrix with the form of:

$$|\psi\rangle = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_{n-1} \\ z_n \end{bmatrix}$$

With the complex numbers $(z_1, z_2, \dots, z_{n-1}, z_n)$ as its elements. A vector written as $|\psi\rangle$ is named *ket*.

Addition of a pair of the vectors on a Hilbert space it defined by 1:

$$|\psi\rangle + |\varphi\rangle = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} + \begin{bmatrix} \varphi_1 \\ \vdots \\ \varphi_n \end{bmatrix}$$

Moreover, there is a scalar multiplication defined by:

$$z |\psi\rangle = z \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} = \begin{bmatrix} z\psi_1 \\ \vdots \\ z\psi_n \end{bmatrix}$$

¹The vectors on this definition have their elements represented with their label and a subscript e.g. the vector $|\psi\rangle$ as an element ψ_i in it and its first element is ψ_1 . This notation is followed from now on.

Where z is a scalar and $|\psi\rangle$ a vector. Note that each element of the vector is multiplied by the scalar.

Because Hilbert spaces are complex spaces they have a conjugate defined for scalars as: For a complex scalar z=a+bi its conjugate z^* is equal to a-bi. This notion can be extended for both vectors and matrices taking the conjugate of all the entries:

$$|\psi\rangle^* = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} * = \begin{bmatrix} \psi_1^* \\ \vdots \\ \psi_n^* \end{bmatrix}$$

$$A^* = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_m n \end{bmatrix}^* = \begin{bmatrix} A_{11}^* & \dots & A_{1n}^* \\ \vdots & \ddots & \vdots \\ A_{m1}^* & \cdots & A_m n^* \end{bmatrix}$$

With $|\psi\rangle$ being a vector and A being a matrix of dimension $m \times n$.

Another important concept is the transpose represented with a superscript T that 'flips' a vector or a matrix. A column vector with dimension n,1 becomes a row vector with dimension $1, n^2$:

$$|\psi\rangle^T = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix}^T = \begin{bmatrix} \psi_1 & \dots & \psi_n \end{bmatrix}$$

The same holds for matrices, a transposed $m \times n$ matrix becomes a $n \times m$ matrix. For example:

$$A^{T} = \begin{bmatrix} 2 & 3 \\ 6 & 4 \\ 2 & 5 \end{bmatrix}^{T} = \begin{bmatrix} 2 & 6 & 2 \\ 3 & 4 & 5 \end{bmatrix}$$

The combination of the complex conjugate and the transpose is named the Hermitian conjugate, written as a superscript \dagger . For a vector $|\psi\rangle$ its Hermitian conjugate $|\psi\rangle^{\dagger}$ is:

$$|\psi\rangle^{\dagger} = (|\psi\rangle^*)^T = \begin{bmatrix} \psi_1^* & \dots & \psi_n^* \end{bmatrix} = \langle \psi |$$

This equivalence works both ways: $|\psi\rangle^{\dagger} = \langle \psi|$ and $\langle \psi|^{\dagger} = |\psi\rangle$.

²In reality column vectors are matrices of dimension n,1 but I have been omitting the 1. When referring to the dimensions of any vector I am going to say just a number, nonetheless, I will also specify the type of vector -a column or a row one-.

The Hermitian conjugate of a column vector $|\psi\rangle$ is named *bra* or dual vector. On Dirac notation is written as $\langle\psi|$.

2.1.2 Linear Operators

To operate with vectors and do operations on them matrices are used. Matrices are also named linear maps or linear operators, which are names that illustrate better what they do. The formal definition of a linear operator can be quite complicated, thus, in this section I am going to explained in more mundane terms.

Put it simply, a linear operator transforms a vector onto another vector, those two vectors can be on different spaces or not. More formally, for a vector $|v\rangle$ on the space V and a vector $|w\rangle$ on the space W, a linear operator A between this two vectors, performs the action:

$$A|v\rangle = |w\rangle$$

In other words, it maps an element of the vector space V to an element of the vector space W. Linear operators must preserve the following operations:

1. Vector addition:

For the vectors $|\psi\rangle$ and $|\varphi\rangle$ on the same vector space, and the linear operator A:

$$A(|\psi\rangle + |\varphi\rangle) = A|\psi\rangle + A|\varphi\rangle$$

2. Scalar multiplication:

For the vector $|\psi\rangle$, the scalar z and the linear operator A:

$$A(z|\psi\rangle) = zA|\psi\rangle$$

These affirmations have to be true for all vectors and all scalars on the spaces that the linear operator acts upon. Note that a linear operator doesn't have to be a matrix necessarily, for example, derivatives and integrals are linear operators, you can check easily that they follow the criteria specified above. However, they are usually applied to functions, although, it is possible to make derivatives and integrals with matrices.³

Matrices are just the matrix representation of a linear operator

³Don't you worry, I am definitely going to do that, and I hope you are as excited as I am :D.

2.1.2.1 Types of linear operators On the current section, I am going to cover the basic types of linear operators that are indispensable for the following theory on this chapter and the experimental work.

1. Zero operator

The zero operator Every vector space has a zero vector that in Dirac notation is represented by 0, since, $|0\rangle$ is belong to something completely different on QC and QI. The zero vector is such that for any other vector $|\psi\rangle$ and any scalar z: $|\psi\rangle + 0 = |\psi\rangle$ and z0 = 0. Note that the zero operator is also represented as 0 and its defined as the operator that maps all vectors to the zero vector: 0 $|\psi\rangle = 0$.

2. Inverse matrix

A squared matrix⁴ A is called invertible if there exist a matrix A^{-1} such that $AA^{-1} = A^{-1}A$. A^{-1} is the inverse matrix of A. The fastest way to see if a square matrix is invertible is to check if it has a non-zero determinant.

3. Identity operator

For any vector space V there exist an identity operator I that is defined as $I |\psi\rangle = |\psi\rangle$, this operator doesn't do anything to the vectors that it is applied to. Note that for any matrix A and its inverse A^{-1} is true that $AA^{-1} = I$.

4. Unitary operator

A unitary operator is any operator that doesn't change the norm of the vectors that it is applied to, moreover, a matrix A is unitary if $AA^{\dagger}=I$. To convert any operator to unitary all its entries are divided by the norm of the operator.

5. Hermitian operators

A Hermitian operator or self-adjoint operator is any operator that its Hermitian conjugate is itself $A=A^{\dagger}$. Another thing to point out, is that there exist a unique operator A on a Hilbert space. Such that for any vectors $|\psi\rangle$ and $|\varphi\rangle$:

$$\langle \psi | (A | \varphi \rangle) = (A^{\dagger} \langle \psi |) | \varphi \rangle$$

This operator is known as the adjoint or Hermitian conjugate of A.

 $^{^4}$ A square matrix is a matrix with dimensions $n \times n$.

2.1.3 Inner Product and Outer Product

2.1.3.1 Inner product A dual vector $\langle \psi |$ and a vector $| \varphi \rangle$ combined form the inner product $\langle \psi | \varphi \rangle$ which is an operation that takes two vectors of the same space as input and produces a complex number as output:

$$\langle a|b\rangle = a_1b_1 + a_2b_2 + \dots + a_{n-1}b_{n-1} + a_nb_n = z$$

With $z, a_i, b_i \in \mathbb{C}$. When referring to an inner product I will often say 'the inner product of two vectors' when in reality is an operation between a dual vector and a vector.

The equivalent to this product on a 2 dimensional real space \mathbb{R}^2 is the dot product, which is also expressed as:

$$\langle a|b\rangle = ||a\rangle||_2 \cdot ||b\rangle||_2 \cos \theta \tag{2.1}$$

With $\|\cdot\|_2$ being the ℓ^2 norm defined by $\||\psi\rangle\|_2 = \sqrt{\psi_1^2 + \ldots + \psi_n^2}$ and θ being the angle between the vectors $|a\rangle$ and $|b\rangle$. As I said the equation (2.1) is equivalent to the inner product, however, from what I have seen, it is not widely used when working in high dimensional spaces because interpreting θ as an angle doesn't make sense when referring to vectors that have more than 2 dimensions. Instead, I have seen more often the inner product presented in its geometrical representation⁵ as the product between one row vector and one column vector:

$$\langle a|b\rangle = \begin{bmatrix} a_1...a_n \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

I have already defined the ℓ_2 norm as the square root of the sum of the squared entries of a vector:

$$\||a\rangle\|_2 = \sqrt{\sum_i a_i^2}$$

⁵The exact details of the geometrical representation of matrices and vectors are out of the scope of this work, even so, it gives a clear and intuitive way of looking at vectors and vector spaces [citation].

Nonetheless, the more common definition is based upon the inner product. As you can see the inner product of a vector by itself is the sum of the squared entries:

$$\langle a|a\rangle = a_1 a_1 + \dots + a_n a_n = a_1^2 + \dots + a_n^2 = \sum_i a_i^2$$

Thus, the norm can be defined as the square root of the inner product of a vector:

$$\||a\rangle\|_2 = \sqrt{\langle a|a\rangle} \tag{2.2}$$

When the norm is applied to a 2 dimensional vector you can see that is the same as the length of that vector, that is because norm and length are the same concepts, however, the norm is the generalized length that can be applied to a vector of any dimension.

From what I understand some properties of the length of a two dimensional vector do not hold with the norm of a vector that has more than 2 dimensions. In other words, the norm behaves in similar ways like the distance from the origin (which is the length), thus they are not the exact same thing. Moreover, there are different types of norm⁶ that are used in different types of scenarios. That is why I am referring to a ℓ^2 norm, a specific type of norm that is also named Euclidean norm which is used to define the ℓ^2 distance or Euclidean distance, widely used to measure the distance of two points in a 2D space or a 3D space in high school. [citation]

2.1.3.2 Properties of the Inner Product The basic properties of the inner product are as follows:

- 1. Is linear in the second argument $(z_1 \langle a| + z_2 \langle c|) |b\rangle = z_1 \langle a|b\rangle + z_2 \langle c|b\rangle$
- 2. Conjugate symmetry $\langle a|b\rangle = (\langle b|a\rangle)^*$
- 3. $\langle a|a\rangle$ is non-negative and real, except in the case of $\langle a|a\rangle=0 \Leftrightarrow |a\rangle=0$

⁶But not different types of length, that I know of at least.

2.1.3.3 Orthonormal and orthogonal vectors From the concept of norm comes the concepts a pair of orthogonal vectors and a pair of orthonormal vectors⁷. Looking at the equation (2.2) we can see that if the inner product of a vector is one, the norm of this vector is also one. A vector that has norm one is named a unit vector. Therefore, if the inner product of a vector is one, that vector is a unit vector.

A pair of non-zero vectors are orthogonal if their inner product is zero. For two non-zero 2 dimensional vectors, if their inner product is equal to zero, you can see that they are perpendicular to each other by looking at equation (2.1):

For $|a\rangle$ and $|b\rangle \neq 0$:

If
$$\langle a|b\rangle = 0$$
 then: $||a\rangle||_2 \cdot ||b\rangle||_2 \cos \theta = 0$

Because $|a\rangle$ and $|b\rangle$ are non-zero vectors, their norms can't be zero.

Thus the remainder term $\cos\theta$ is equal to zero.

Therefore, the angle
$$\theta$$
 as to be $\frac{\pi}{2}$.

However, thinking that perpendicularity and orthogonality are the same concepts is a mistake, since, it only holds when looking at 2 dimensional vectors. As with norm and length, orthogonality is the generalized concept of perpendicularity that works for high dimensional vectors.

When we mix the concepts of unit vector and orthogonal vectors we arrive at the term orthonormality [citation]. A pair of non-zero vectors are orthonormal when both are unit vectors and there are orthogonal to each other:

$$|a\rangle$$
 and $|b\rangle$ are othornormal if
$$\left\{ egin{array}{l} \langle a|b\rangle = 0 \\ \langle a|a\rangle = 1 \\ \langle b|b\rangle = 1 \end{array} \right.$$

Orthonormal vectors are important, they are broadly used in quantum computation as well as quantum mechanics because they form the basis for the vector spaces on which the quantum states are located.

One thing to point out is that I have been talking about a pair of vectors when referring to orthonormal vectors, however, orthonormality can be extended to a

maybe introduce them before if you talk about basis later on

⁷Funny note, when I encountered these two terms for the first time in QC and QI [citation], I taught they were the same thing and a week passed until I realized. It was such a difficult mess to understand everything else with these two terms confused.

set of vectors. If a set has all unit vectors and the vectors are orthogonal to each other, the set is orthonormal. The set of vectors $B = \{|\beta_1\rangle\,, |\beta_2\rangle\,, ..., |\beta_{n-1}\rangle\,|\beta_n\rangle\}$ is orthonormal if $\langle\beta_i|\beta_i\rangle = \delta_{ij} \forall i,j$ [citation] where δ_{ij} is the Kronecker delta defined as :

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

2.1.3.4 Outer product The outer product is a function that takes two vectors -expressed as $|a\rangle \langle b|$, with $|a\rangle$ and $|b\rangle$ being vectors- and produces an linear operator as output. Unlike the inner product, there is no analog for the outer product on the mathematics taught in high school⁸, and it is a bit difficult to understand it as it can take two vectors from different spaces as input. It is defined as follows:

For a vector $|v\rangle$ and $|v'\rangle$ of dimensions m and a vector $|w\rangle$ of dimension n. The output is a linear operator A of dimensions $m \times n$ in the space $M_{m \times n}$:

$$|v\rangle\langle w|=A$$
 with $A\in \mathrm{Mat}_{m\times n}$.

Whose action is defined by:

$$(|v\rangle\langle w|)|v'\rangle \equiv |w\rangle\langle v|v'\rangle = \langle v|v'\rangle|w\rangle \tag{2.3}$$

From equation (2.3) the usefulness and meaning of the outer product are hard to comprehend, so I will look at the way to compute it next to clarify how it works. For two vectors $|a\rangle$ and $|b\rangle$ of dimensions m and n respectively, their outer product is computed multiplying each element of $|a\rangle$ by each element of $|b\rangle$ forming a matrix of size $m \times n$:

$$|a\rangle\langle b| = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_n \\ a_2b_1 & a_2b_2 & \cdots & a_2b_n \\ \vdots & \vdots & \ddots & \vdots \\ a_mb_1 & a_mb_2 & \cdots & a_mb_n \end{bmatrix}$$

The usefulness of the outer product will be shown in future sections.

⁸The analog of the inner product would be the dot product.

2.1.4 Tensor product

The last product to mention is the tensor product, represented with the symbol \otimes . This product is used to create larger vector spaces by combining smaller vector spaces. The formal explanation of this concept is quite difficult, so I will focus on explaining the way to compute it by using the matrix representation of this product, named the Kronecker product.

For a $m \times n$ matrix A and a $p \times q$ matrix B the output of their Kronecker product is a $pm \times qn$ matrix:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{bmatrix}$$

$$= \begin{bmatrix} a_{11}b_{11} & a_{11}b_{12} & \cdots & a_{11}b_{1q} & \cdots & \cdots & a_{1n}b_{11} & a_{1n}b_{12} & \cdots & a_{1n}b_{1q} \\ a_{11}b_{21} & a_{11}b_{22} & \cdots & a_{11}b_{2q} & \cdots & \cdots & a_{1n}b_{21} & a_{1n}b_{22} & \cdots & a_{1n}b_{2q} \\ \vdots & \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ a_{11}b_{p1} & a_{11}b_{p2} & \cdots & a_{11}b_{pq} & \cdots & \cdots & a_{1n}b_{p1} & a_{1n}b_{p2} & \cdots & a_{1n}b_{pq} \\ \vdots & \vdots & & \vdots & \ddots & \vdots & & \vdots \\ a_{m1}b_{p1} & a_{m1}b_{p2} & \cdots & a_{m1}b_{pq} & \cdots & \cdots & a_{mn}b_{p1} & a_{mn}b_{p2} & \cdots & a_{mn}b_{pq} \\ \vdots & \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ a_{m1}b_{p1} & a_{m1}b_{p2} & \cdots & a_{m1}b_{pq} & \cdots & \cdots & a_{mn}b_{p1} & a_{mn}b_{p2} & \cdots & a_{mn}b_{pq} \end{bmatrix}$$

Note that $a_{ij}B$ is a scalar multiplication by a matrix, with a_{ij} being the scalar and B being the matrix.

Here is a clearer example with two 2×2 matrices, note that each entry of the first matrix is multiplied by the second matrix:

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \otimes \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} = \begin{bmatrix} 1 \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} & 2 \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} \\ 3 \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} & 4 \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} \end{bmatrix}$$

$$= \begin{bmatrix} 1 \times 0 & 1 \times 5 & 2 \times 0 & 2 \times 5 \\ 1 \times 6 & 1 \times 7 & 2 \times 6 & 2 \times 7 \\ 3 \times 0 & 3 \times 5 & 4 \times 0 & 4 \times 5 \\ 3 \times 6 & 3 \times 7 & 4 \times 6 & 4 \times 7 \end{bmatrix} = \begin{bmatrix} 0 & 5 & 0 & 10 \\ 6 & 7 & 12 & 14 \\ 0 & 15 & 0 & 20 \\ 18 & 21 & 24 & 28 \end{bmatrix}$$

One important piece of notation to take into account is \otimes , used to represent the equivalent of the sum (noted with \sum), but instead of addition the Kronecker product is used. In other words \otimes denotes the Kronecker product of a finite number of terms. To clarify here's an example with the identity matrix:

With \mathbb{I} as the matrix $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and n as a power of 2:

$$\mathbb{I}_n = \bigotimes^{\log_2 n} \mathbb{I}$$

Here is the case for n = 8:

$$\mathbb{I}_{8} = \bigotimes^{\log_{2} 8} \mathbb{I} = \bigotimes^{3} \mathbb{I} = \mathbb{I} \otimes \mathbb{I} \otimes \mathbb{I} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The Kronecker product also works for vectors in the same way, with a scalar-vector multiplication:

For the vectors $|\psi\rangle$ and $|\varphi\rangle$ of dimensions n and m respectively:

$$|\psi\rangle \otimes |\varphi\rangle = \begin{bmatrix} \psi_1 |\varphi\rangle \\ \psi_2 |\varphi\rangle \\ \vdots \\ \psi_m |\varphi\rangle \end{bmatrix} = \begin{bmatrix} \psi_1 \varphi_1 \\ \psi_1 \varphi_2 \\ \vdots \\ \psi_n \varphi_m \\ \vdots \\ \vdots \\ \psi_n \varphi_1 \\ \psi_n \varphi_2 \\ \vdots \\ \psi_n \varphi_m \end{bmatrix}$$

Note that the Kronecker product can also be taken between a vector and a matrix or vise-versa, however this form isn't as common as the other two.

2.1.4.1 Properties of the Tensor Product The basic properties of the tensor product are as follows:

1. Associativity:

$$A \otimes (B + C) = A \otimes B + A \otimes C$$
$$(zA) \otimes B = A \otimes (zB) = z(A \otimes B)$$
$$(A \otimes B) \otimes C = A \otimes (B \otimes C)$$
$$A \otimes 0 = 0 \otimes A = 0$$

2. Non-commutative 9:

$$A \otimes B \neq B \otimes A$$

2.1.5 Trace

The trace of a matrix is just the sum of the elements on the main diagonal, the one that goes from top to bottom and left to right.

⁹One cool thing is that $A \otimes B$ and $B \otimes A$ are permutation equivalent: $\exists P, Q \Rightarrow A \otimes B = P(B \otimes A)Q$ where P and Q are permutation matrices.

Here's a matrix A with its main diagonal marked:

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

And its trace, denoted by Tr[A] is:

$$Tr[A] = 1 + 1 + 1 = 3$$

More formally, the trace of a n-dimensional squared matrix A is:

$$Tr[A] = \sum_{i=1}^{n} a_{ii} = a_{11} + a_{22} + \dots + a_{nn}$$

The trace of a matrix as the following properties:

1. Linear operator:

Because the trace is a linear mapping, it follows that:

Tr[A+B] = Tr[A] + Tr[B] and Tr[zA] = z Tr[A], for all squared matrices A and B and all scalars z.

2. Trace of a Kronecker product:

$$Tr[A \otimes B] = Tr[A] Tr[B]$$

3. Transpose has the same trace:

$$\operatorname{Tr}[A] = \operatorname{Tr}[A^T]$$

4. Trace of a product is cyclic:

For a $m \times n$ matrix A and a $n \times m$ matrix B:

$$Tr[AB] = Tr[BA]$$

One very useful way to compute the trace of an operator is through the Gram-Schmidt procedure 10 and an outer product. Using Gram-Schmidt to represent the unit vector $|\psi\rangle$ with an orthonormal basis $|i\rangle$ which includes $|\psi\rangle$ as the first element, is true that:

$$\operatorname{Tr}[A|\psi\rangle\langle\psi|] = \sum_{i} \langle i|A|\psi\rangle\langle\psi|i\rangle = \langle\psi|A|\psi\rangle$$

¹⁰See A.1 for the definition of the Gram-Schmidt procedure.

2.2 Quantum Computation

Chapter 3

Experimental Work

Chapter 4

Conclusions

Bibliography

Appendices

Appendix A

More Linear Algebra

I have wrote many pages of linear algebra theory, but that wasn't enough. So here we go, I guess.

A.1 Gram-Schmidt Procedure

The Gram–Schmidt procedure is a method used to produce orthonormal basis for a vectors space. For a d-dimensional inner product vector space V with a basis vectors set $|v_1\rangle$, \cdots , $|v_d\rangle$, we can define a new orthonormal basis set $\{|u\rangle\}$. The first element of that set is $|u_1\rangle=|v_1\rangle$ / $||v_1\rangle||$, with the following element $|v_{k+1}\rangle$ being:

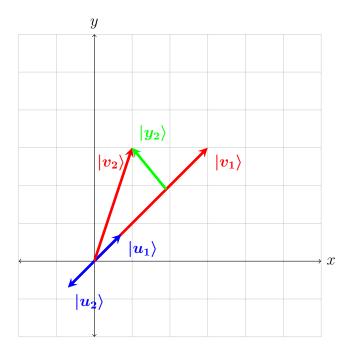
$$|u_{k+1}\rangle = \frac{|v_{k+1}\rangle - \sum_{i=1}^{k} \langle u_i | v_{k+1}\rangle |u_i\rangle}{\left\||v_{k+1}\rangle - \sum_{i=1}^{k} \langle u_i | v_{k+1}\rangle |u_i\rangle\right\|}$$

For k in the interval $1 \le k \le d-1$.

If we follow the above for each k in $1 \le k \le d-1$, we obtain the new vector set $|u_1\rangle, \cdots, |u_d\rangle$ that is a valid orthonormal basis for the space V. The created vector set must have the same span¹ as the previous one to be a valid basis for the space V:

$$span(\{|v\rangle\}) = span(\{|v\rangle\}) = V$$

¹The span of a set of vectors is all the possible linear combinations that come from those vectors.



Note that the span of the basis set is the definition of the space. In other words, every vector in V can be represented as a linear combination of the basis vectors.

To get at some intuition let's look at the case for k = 1:

$$|u_2\rangle = \frac{|v_2\rangle - \langle u_1|v_2\rangle |u_1\rangle}{\||v_2\rangle - \langle u_1|v_2\rangle |u_1\rangle\|}$$

We can see that the vector $|u_2\rangle$ is defined by the subtraction of the vector $|v_2\rangle$ by the projection² of $|v_2\rangle$ onto $|v_1\rangle$. Which is equivalent for the projection of $|v_2\rangle$ onto $|u_1\rangle$, remember that $|u_1\rangle$ is just $|v_1\rangle$ normalized. Therefore we have:

The proof that is an orthonormal basis is quite simple: We can see immediately that the components of $\{|u\rangle\}$ are unit vectors because they are normalized (the vectors $|v_{k+1}\rangle - \sum_{i=1}^k \langle u_i|v_{k+1}\rangle \, |u_i\rangle$ are divided by their norm). And we can se that they are orthogonal by checking that the inner product of non-equal vectors in the set is 0:

For
$$k=1$$
:
$$|u_2\rangle=\frac{|v_2\rangle-\langle u_1|v_2\rangle\,|u_1\rangle}{\||v_2\rangle-\langle u_1|v_2\rangle\,|u_1\rangle\|}$$

²The way to project the vector $|a\rangle$ onto $|b\rangle$ is: $\langle b|a\rangle |b\rangle$.

Then the inner product with $|v_1\rangle$ is:

$$\langle u_1 | u_2 \rangle = \langle u_1 | \left(\frac{|v_2\rangle - \langle u_1 | v_2 \rangle | u_1 \rangle}{\||v_2\rangle - \langle u_1 | v_2 \rangle | u_1 \rangle\|} \right)$$

$$= \frac{\langle u_1 | v_2 \rangle - \langle u_1 | v_2 \rangle \langle u_1 | u_1 \rangle}{\||v_2\rangle - \langle u_1 | v_2 \rangle | u_1 \rangle\|}$$

$$= 0$$

By induction we can see that for $j \leq d$, with d being the dimension of the vector space:

$$\langle u_{j}|u_{n+1}\rangle = \langle u_{j}|\left(\frac{|v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle |u_{i}\rangle}{\||v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle |u_{i}\rangle\|}\right)$$

$$= \frac{\langle u_{j}|v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle \langle u_{j}|u_{i}\rangle}{\||v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle |u_{i}\rangle\|}$$

$$= \frac{\langle u_{j}|v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle |u_{i}\rangle\|}{\||v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle |u_{i}\rangle\|}$$

$$= \frac{\langle u_{j}|v_{n+1}\rangle - \langle u_{j}|v_{n+1}\rangle}{\||v_{n+1}\rangle - \sum_{i=1}^{n} \langle u_{i}|v_{n+1}\rangle |u_{i}\rangle\|}$$

$$= 0$$

All of this doesn't seem straightforward at first but remember that the inner product of two orthogonal vectors is zero, and the inner product between the same unit vector is one.

A.2 Dirac Notation Crash Course

On the following table there is a quick summary important mathematical concepts of linear algebra expressed in Dirac Notation³.

³The notation used for the complex vector spaces and complex number space are not standard Dirac Notation, but I included them in the table to explain what they mean.

Notation	Description
\overline{z}	Complex number
z^*	Complex conjugate of the a complex number z . $(a+bi)^* = (a-bi)$
$ \psi angle$	Vector with label ψ . Known as ket
$ \psi\rangle^T$	Transpose of vector $ \psi angle$
$ \psi angle^\dagger$	Hermitian conjugate of vector. $ \psi\rangle^{\dagger}=(\psi\rangle^{T})^{*}$
$\langle \psi $	Dual vector to $ \psi\rangle$. $ \psi\rangle = \langle\psi ^{\dagger}$ and $\langle\psi = \psi\rangle^{\dagger}$. Known as <i>bra</i>
$\langle \varphi \psi \rangle$	Inner product of vectors $\langle \varphi $ and $ \psi \rangle$
$ \varphi\rangle\langle\psi $	Outer product of vectors $\langle \varphi $ and $ \psi \rangle$
$ \psi angle\otimes arphi angle$	Tensor product of vectors $ arphi angle$ and $ \psi angle$
0	Zero vector and zero operator
\mathbb{I}_n	Identity matrix of dimension n
\mathbb{C}_n	Complex vector space of dimension n
\mathbb{C}_1 or \mathbb{C}	Complex number space

A.3 More on the Partial Trace