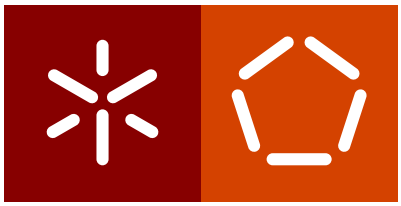

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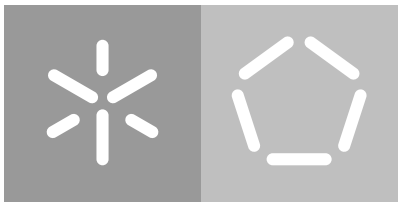

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Master dissertation
Master Degree in Física da Informaçao

Dissertation supervised by
Luís Barbosa
Bruno Chagas

November 2020

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Write acknowledgements here

ABSTRACT

Implementation of staggered quantum walks in qiskit.

RESUMO

Pensar no que escrever aqui. Hello!

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QUANTUM COMPUTING

2.1 GROVER'S ALGORITHM

Searching through an unstructured database is a task classically achieved by exhaustively evaluating every element in the database. Assume there exists a black box (oracle) that can be asked to find out if two elements are equal. Since we're looking for a specific element in a database of size N, we'd have to query the oracle on average $\frac{N}{2}$ times, or in the worst case N times.

Grover's algorithm, presented in Grover (1996), comes as a quantum alternative to this type of problems, taking advantage of superposition by increasing desirable states' amplitudes through a process called *amplitude amplification*. This method has a quadratic gain over the classical counterpart Boyer et al. (1998), being able to find a target element in expected time $\mathcal{O}(\sqrt{N})$.

Let us now expand on the inner workings of the black box. We start by focusing on searching indexes instead of directly evaluating the element and we assume $N = 2^n$, n being a positive integer. We can now define a function $f : \{0, 1, ..., N-1\}$ that returns 1 when evaluating the desired (marked) element and 0 otherwise. Since this function is to be applied to a quantum system, we must build a unitary operator $\mathcal{O}$

$$\mathcal{O} |x\rangle |i\rangle = |x\rangle |i \oplus f(x)\rangle . \tag{1}$$

where $|x\rangle$ is the index register, $\oplus$ is the binary sum operation and $|i\rangle$ is a qubit that is flipped if $f(x) = 1$.

The action of the oracle on state $|0\rangle$ will be

$$\mathcal{O} |x\rangle |0\rangle = \begin{cases} |x_0\rangle |1\rangle , & \text{if } x = x_0 \\ |x\rangle |0\rangle , & \text{otherwise.} \end{cases} \tag{2}$$

where x_0 is the marked element. More generically, $\mathcal{O}$ can be written as

$$\mathcal{O} |x\rangle = (-1)^{f(x)} |x\rangle . \tag{3}$$

This offers a bit of insight into the oracle, it *marks* the solutions to the search problem by applying a phase shift to the solutions. The question now is, what is the procedure that determines a solution x_0 using $\mathcal{O}$ the minimum number of times? The answer lies in the amplitude amplification section of Grover's search, starting with the creation of a uniform superposition

$$|\Psi_0\rangle = H^{\otimes n} |x\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle \tag{4}$$

where $H^{\otimes n}$ is the *Hadamard* operator applied to an arbitrary number of states.

If we were to measure $|x\rangle$ at this point, the superposition would collapse to any of the base states with the same probability $\frac{1}{N} = \frac{1}{2^n}$, which means that on average, we'd need to try $N = 2^n$ times to guess the correct item. This is where amplitude amplification comes into effect, by means of a second unitary operator

$$\mathcal{D} = (2 |\Psi_0\rangle \langle\Psi_0| - I) = H^{\otimes n}(2 |0\rangle \langle 0| - I)H^{\otimes n} \tag{5}$$

This operator applies a conditional phase shift, with every computational basis state except $|0\rangle$ receiving a phase shift. This can also be described as the *inversion about the mean*, for a state of arbitrary amplitudes

$$|\phi\rangle = \sum_{k=0}^{N-1} \alpha_k |k\rangle \tag{6}$$

the action of $\mathcal{D}$ on state ϕ will be

$$\mathcal{D} |\phi\rangle = \sum_{k=0}^{N-1} (-\alpha_k + 2\langle\alpha\rangle) |k\rangle \tag{7}$$

where $\langle\alpha\rangle$ is the average of α_k

$$\langle\alpha\rangle = \frac{1}{N} \sum_{k=0}^{N-1} \alpha_k |k\rangle \tag{8}$$

The evolution operator that performs one step of the algorithm is then

$$\mathcal{U} = \mathcal{D}\mathcal{O} \tag{9}$$

and after t steps the state of the system is

$$|\Psi(t)\rangle = \mathcal{U}^t |\Psi_0\rangle . \tag{10}$$

2.1.1 *One marked element*

The optimal number of steps is, as aforementioned, proportional to $\sqrt{N}$. More precisely, if there's only one solution, maximum probability can be reached in *approximately* $\frac{\pi}{4}\sqrt{N}$ iterations. In order to show that this is the case, an iteration will be formally defined here as the process that transforms the state

$$|\Psi(k,l)\rangle = k\,|i_0\rangle + \sum_{i\neq i_0} l\,|i\rangle \tag{11}$$

into state $\left|\Psi(\frac{N-2}{N}k + \frac{2(N-1)}{N}l, \frac{N-2}{N}l - \frac{2}{N}k)\right\rangle$. Numbers l and k are real numbers that statisfy $k^2 + (N-1)l^2 = 1$. Running m iterations over state $|\Psi_0\rangle$ will eventually lead to state $|\Psi_j\rangle = |\Psi(k_j, l_j)\rangle$ after the $j-th$ iteration, where $k_0 = l_0 = \frac{1}{\sqrt{N}}$ and

$$\begin{cases} k_{j+1} = \frac{N-2}{N}k_j + \frac{2(N-1)}{N}l_j \\ l_{j+1} = \frac{N-2}{N}l_j + \frac{2}{N}k_j. \end{cases} \tag{12}$$

After the last iteration, the system will be in state $|\Psi_m\rangle$ with a certain amplitude. If that amplitude corresponds to the marked element x_0, then it is said that the algorithm was successful.

Grover (1996) proves that there exists a value of $m < \sqrt{2N}$ such that the probability of success is at least $\frac{1}{2}$. However the probability of success does not linearly increase with the number of iterations, in fact for $m = \sqrt{2N}$ the system will succeed less that 1 in 10 times. Boyer et al. (1998) argues that an explicit value of m is needed, and it is achieved by finding a closed form formula for k_j and l_j. The first step is to define an angle θ so that $\sin^2\theta = \frac{1}{N}$, and equation 12 will become

$$\begin{cases} k_{j+1} = \sin\left((2j+1)\theta\right) \\ l_{j+1} = \frac{1}{\sqrt{N-1}}\cos\left((2j+1)\theta\right). \end{cases} \tag{13}$$

In order to maximize the probability of success, one must find a value of m so that $k_m = 1$ and l_m is as close to 0 as possible. The value of k after m iterations will be at it's maximum when $\sin\left((2m+1)\theta\right) = \frac{\pi}{2}$, and solving the trigonometric equation leads to a value of $m = \frac{\pi - 2\theta}{4\theta}$. Conversely, $l_{\widetilde{m}} = 0$ when $\widetilde{m} = \frac{\pi-2\theta}{4\theta}$ for an integer number of $\widetilde{m}$. Setting m to the nearest lower integer of $\frac{\pi}{4\theta}$ will lead to

$$|m - \widetilde{m}| \leq \frac{1}{2} \iff |(2m+1)\theta - (2\widetilde{m}-1)\theta| \leq \frac{\pi}{2}. \tag{14}$$

By definition, $(2\widetilde{m}+1)\theta = \frac{\pi}{2}$ which means that $|\cos((2m+1)\theta)| \leq |\sin\theta|$. The probability of failure after m iterations can then be written as

$$(N-1)l_m^2 = \cos^2((2m+1)\theta) \leq \sin^2\theta = \frac{1}{N}. \tag{15}$$

Failure decreases as the number of elements increases. The run time of the algorithm will be

$$m \leq \frac{\pi}{4\theta} \leq \frac{\pi}{4}\sqrt{N} \tag{16}$$

since $\theta \geq \sin\theta = \frac{1}{\sqrt{N}}$. This means that, for a large N, the number of iterations that maximizes the probability of success will be very close to $\frac{\pi}{4}\sqrt{N}$.

Figure 1 was obtained by coding the apropriate operators as to simulate the system presented in equation 10. The unitary evolution operator was applied approximately

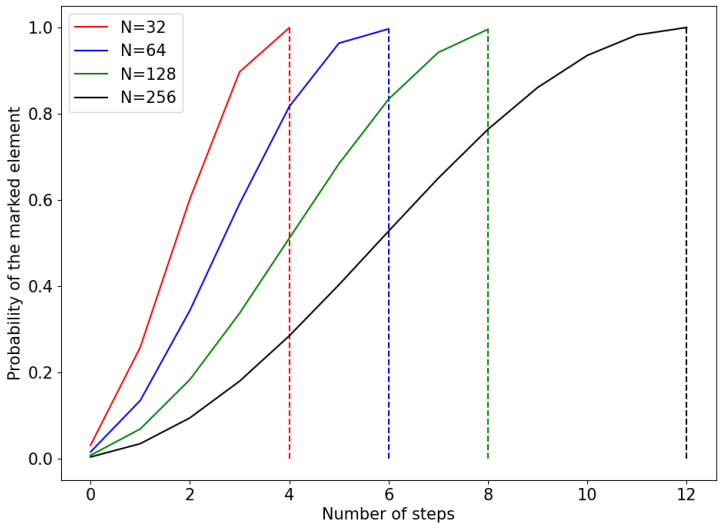

Figure 1: Grover one marked element temp.

$\frac{\pi}{4}\sqrt{N}$ times and the amplitudes associated with those states were stored as a probability distribution. Filtering the probability of the marked element and plotting it against the number of steps, shows that the maximum is indeed reached after the said number of iterations. It also shows that the maximum probability for $N = 16$ is lower than for $N = 128$, which makes sense since the the probability of success is maximized for larger values of N.

2.1.2 *Multiple marked elements*

When there's more than one element marked by the oracle, the number of iterations to achieve maximum probability changes. In fact, the latter part of this section will be used to discuss the case where one single iteration of this algorithm is enough to achieve maximum probability.

Firstly, one must define a set A that is composed of all the marked elements and set B of the remaining. The state from equation 11 will become

$$|\Psi(k,l)\rangle = \sum_{i\in A} k\,|i\rangle + \sum_{x\in B} l\,|x\rangle\,. \tag{17}$$

Assuming t marked elements, iterating over this state will result in

$$\left|\Psi\left(\frac{N-2t}{N}k + \frac{2(N-1)}{N}l, \frac{N-2}{N}l - \frac{2}{N}k\right)\right\rangle. \tag{18}$$

Choosing an angle θ such that $sin^2\theta = \frac{t}{N}$, allows the definition of the amplitudes associated with the states after j iterations

$$\begin{cases} k_j = \frac{1}{\sqrt{t}}\sin\left((2j+1)\theta\right) \\ l_j = \frac{1}{\sqrt{N-t}}\cos\left((2j+1)\theta\right). \end{cases} \tag{19}$$

Similarly to the one solution case, it can be shown that setting the number of iterations

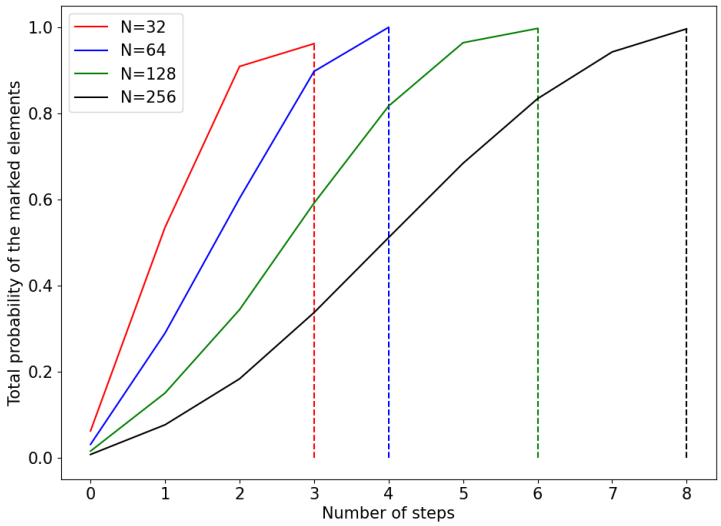

Figure 2: Grover Multiple marked temp.

m, to the nearest lower integer of $\frac{\pi}{4\theta}$ will result in a probability of failure $(N-t)l_m^2 \leq \frac{t}{N}$. Because $\theta \geq \sin\theta = \sqrt{\frac{t}{N}}$ then

$$m \leq \frac{\pi}{4\theta} \leq \frac{\pi}{4}\sqrt{\frac{N}{t}}. \tag{20}$$

In a more practical perspective, if one were to mark two elements of a 64 element set, maximum probability is expected to be reached in approximately 3 steps, since $\lfloor \frac{\pi}{4}\sqrt{\frac{64}{2}} \rfloor = 4$. Similarly for $N = 256$, the number of iterations is rounded to 8, and this can be seen plotted along several other values of N in figure 2. The y-axis is now the sum total probability of the marked elements and the x-axis represents the range of steps that spans from 0 to $\lfloor \frac{\pi}{4}\sqrt{\frac{N}{2}} \rfloor$ for each N. Again, the probability of success approaches 1 as N increases. However, comparing to figure 1, the number of iterations that maximize probability is lower for each N, in agreement with equation 20

2.1.3 *Single-Shot Grover*

3

QUANTUM WALKS

3.1 COINED QUANTUM WALK

Consider a one dimensional walker on top of a line, whose decision to go left or right depends on a coin toss. As expected, the outcome after many iterations of the coin toss is a binomial distribution centered in the starting position. It can be shown that the standard deviation is $\sqrt{t}$, where t is the number of time steps. The one dimensional walk can be abstracted to a graph of any dimension. This is known as the classical random walk and when the graph has its nodes weighted and it's edges directed, it is analogous to a discrete-time Markov chain [1].Você precisa esclarecer desde o início que está falando de uma caminhada clássica aqui, referenciar o livro do renato portugal, por exemplo, sobre o desvio padrão. Se quiser, pode fazer uma simulação clássica ou até mesmo abrir uma seção antes só para isso. Ah, precisa dizer que é uma linha infinita.

In the quantum case, the walker is a quantum system whose position x on the line is described by a vector $|x\rangle$ in Hilbert Space. The next position of the system is determined by a unitary operator, which can be viewed as a quantum coin.O operador unitário não é somente da moeda, precisa falar do espaço do caminhante também The analogy is, if the coin is tossed and rolls "heads", for example, the system transitions to position $|x+1\rangle$, otherwise it advances to $|x-1\rangle$. The Hilbert space of the system is $\mathscr{H} = \mathscr{H}_C \otimes \mathscr{H}_P$, where $\mathscr{H}_C$ is the two-dimensional Hilbert space associated with the "coin" and $\mathscr{H}_P$ is the one-dimensional lattice's Hilbert space. One of the most commonly used coins is the Hadamard operator, which is the one chosen for this example.

The transition from $|x\rangle$ to either $|x+1\rangle$ or $|x-1\rangle$ must be described by a unitary operator, the *shift operator* precisa descrever a moeda também e como ela funciona no unitário e acredito que as equações estejam trocadas

$$\mathcal{S}\,|0\rangle\,|x\rangle = |0\rangle\,|x-1\rangle \tag{21}$$

$$\mathcal{S}\,|1\rangle\,|x\rangle = |1\rangle\,|x+1\rangle \tag{22}$$

1 A Markov chain can be described as a sequence of stochastic events where the the probability of each event depends only on the state of the previous event.

that can also be described by

$$S = |0\rangle\langle 0| \otimes \sum_{x=-\infty}^{x=\infty} |x+1\rangle\langle x| + |1\rangle\langle 1| \otimes \sum_{x=-\infty}^{x=\infty} |x-1\rangle\langle x| . \tag{23}$$

It follows that the operator that describes the dynamics of the quantum walk will be given by Não necessariamente é o Hadamard, poderia ser uma coin qualquer. Você pode explicar também que a H é a sem viés.

$$U = S(H \otimes I). \tag{24}$$

Consider a quantum system located at $|x = 0\rangle$ with coin state $|0\rangle$, for $t = 0$. It's state will be described by

$$|\Psi(0)\rangle = |0\rangle |x = 0\rangle , \tag{25}$$

and after t steps the walker's state will be

$$|\Psi(t)\rangle = U^t |\Psi(0)\rangle , \tag{26}$$

more explicitly

$$|\Psi(0)\rangle \xrightarrow{U} |\Psi(1)\rangle \xrightarrow{U} |\Psi(2)\rangle \xrightarrow{U} (...) \xrightarrow{U} |\Psi(t)\rangle . \tag{27}$$

After applying the Hadamard operator followed by the shift operator twice the respective system states are seria bom especificar que é na moeda, ou até mesmo dizer que o quantum walk consiste da aplicação da moeda e logo em seguida o shift

$$|\Psi(1)\rangle = \frac{|0\rangle |x = -1\rangle + |1\rangle |x = 1\rangle}{\sqrt{2}} \tag{28}$$

$$|\Psi(2)\rangle = \frac{|0\rangle |x = -2\rangle + |1\rangle |x = 0\rangle + |0\rangle |x = 0\rangle - |1\rangle |x = 2\rangle}{2} \tag{29}$$

$$\tag{30}$$

If one were //?// to measure the system after each application of $\mathcal{U}$, it would be expected to see the walker at $x = 1$ 50% of the time and at $x = -1$ for the remainder, after the first iteration (28). Measure the system t times and the result is a binomial probability distribution. The conclusion is that repetitive measurement of a coined quantum walk system reduces to the classical case, which means that any desired quantum behaviour is lost.

It is possible, however, to make use of the quantum correlations between different positions to generate constructive or destructive interference, by applying the Hadamard and shift operators successively without intermediary measurements. The consequences of interference between states are very apparent in

$$|\Psi(3)\rangle = \frac{|1\rangle |x = -3\rangle - |0\rangle |x = -1\rangle + 2(|0\rangle + |1\rangle) |x = 1\rangle + |0\rangle |x = 3\rangle}{2\sqrt{2}}. \tag{31}$$

Even though an unbiased coin was used, this state is not symmetric to the origin and the probability distributions will not be centered in the origin. Moreover, the standard deviation will not be $\sqrt{t}$.Bom, faltou dizer qual o desvio padrão da quantum walk que é t e esse $\sqrt{t}$ é da clássica. Precisa justificar com alguma referência também

The quantum walk is said to be *ballistic* since its standard deviation is proportional to t Venegas-Andraca (2012) meaning exponentially faster hitting times in certain graphs Childs et al. (2002); Farhi and Gutmann (1998) which can be advantageous in problems that involve visiting certain vertices in a graph. There are also studies that show that a quantum walk may have advantages in element distinctness Ambainis (2007) and spatial search Childs and Goldstone (2004) problems. talvez esse parágrafo deva subir, porque você fala de desvio padrão muito antes

In order to study this distribution, a simulation of the coined quantum walk was coded in *Python*. Using the Hadamard coin and the aforementioned initial condition, the resulting probability distribution is:

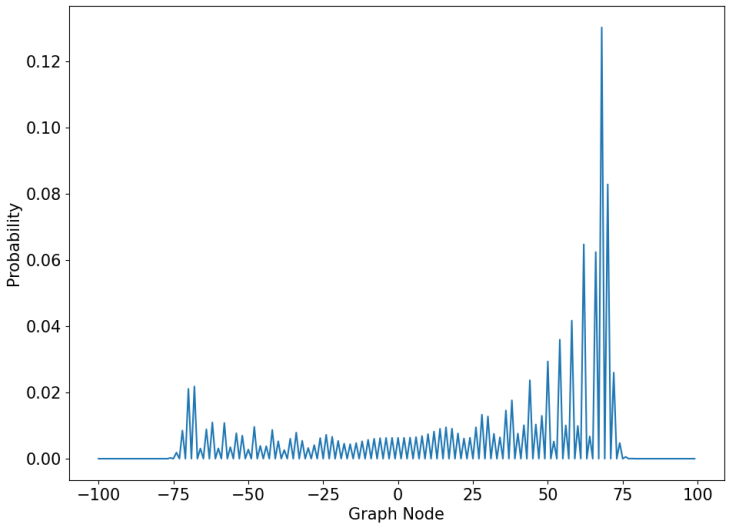

Figure 3: Probability distribution for the coined quantum walk on a line, after 100 steps, with initial condition $|\Psi(0)\rangle = |0\rangle\,|x = 0\rangle$ and the Hadamard coin.

Analyzing the plot, it is noticeable that the distribution is asymmetric, the probability amplitude of finding the walker at the right-hand side is much larger than at the left, with a peak around $x = \frac{100}{\sqrt{2}}$. Regardless of number of steps, this peak is always present (albeit in varying positions), which is to say that the walker can always be found moving in a uniform fashion away from the origin, further confirming the quantum walk's ballistic behaviour. agora penso que um grafo sobre desvio padrão seria bom para ilustrar, porque o desvio padrão foi muito comentado ao longo do texto

Another interesting case study is to find if this behaviour is preserved for a symmetric distribution around the origin. For this purpose, one must first understand where the asymmetry comes from. The Hadamard operator induces a sign flip **[in OU on ?]** não entendi state $|1\rangle$, hence more terms are cancelled when the coin state is $|1\rangle$. Since $|0\rangle$ was defined to induce movement to the right, the result is as shown in 3. It then follows that the initial condition cuidado com a notação embaixo dos kets, e esse sinal negativo é necessário? acredito que não.

$$|\Psi(0)\rangle = -|1\rangle\,|x=0\rangle \tag{32}$$

Will return a mirror image of 3:

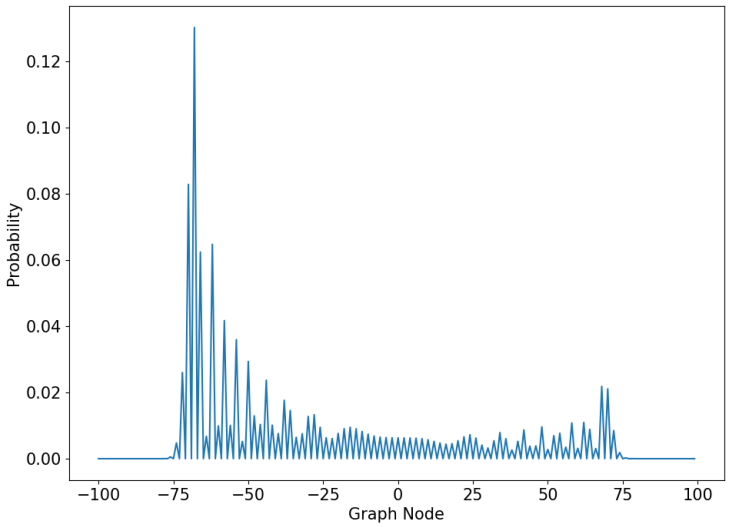

Figure 4: Probability distribution for the coined quantum walk on a line, after 100 steps, with initial condition $|\Psi(0)\rangle = -|1\rangle\,|x=0\rangle$ and the Hadamard coin.

In order to obtain a symmetrical distribution, one must superpose 25 and 33 carefully, as to not cancel terms before the calculation of the probability distribution, by multiplying 33 by the imaginary unit. This works because the entries of the Hadamard operator are real numbers; terms with the imaginary unit will not cancel out with terms without it, thus the walk can proceed to both left and right. The initial condition is then: o sinal pode ser justificado apenas aqui

$$|\Psi(0)\rangle = \frac{|0\rangle - i\,|1\rangle}{\sqrt{2}}\,|x=0\rangle \tag{33}$$

With a correspoding plot:

precisa de um fechamento para esta parte, algo que sumarize os resultados, o que veremos nas próximas partes, etc

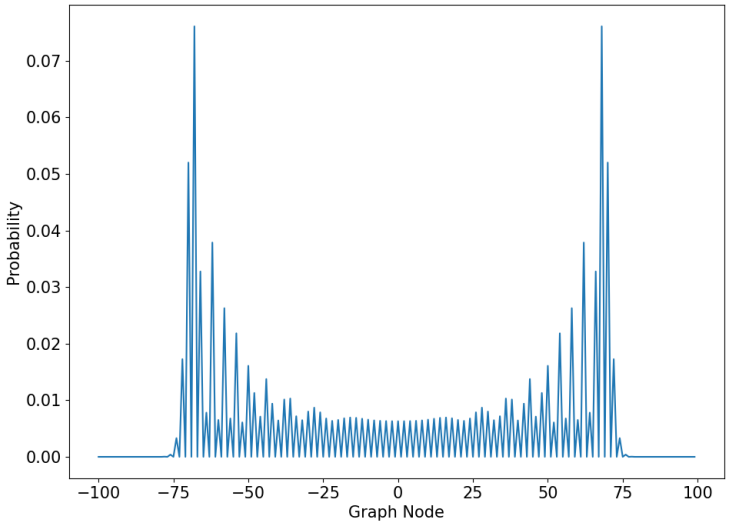

Figure 5: Probability distribution for the coined quantum walk on a line, after 100 steps, with initial condition $|\Psi(0)\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}} |x = 0\rangle$ and the Hadamard coin.

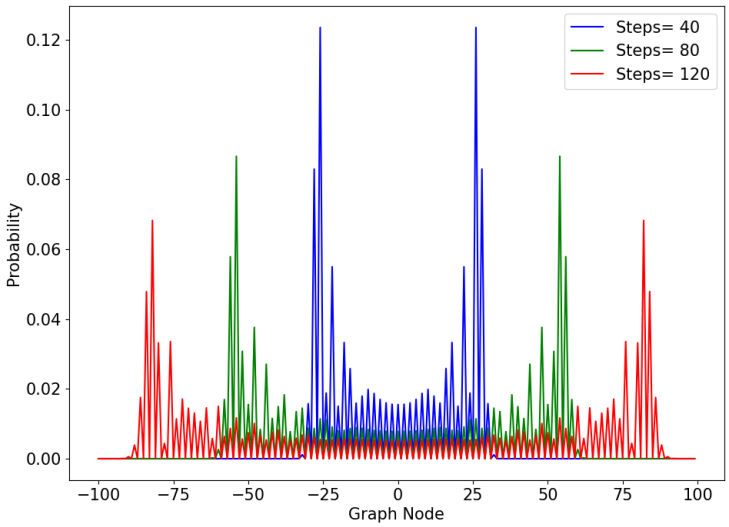

Figure 6: Multiple walks temp

3.2 CONTINUOUS-TIME QUANTUM WALK

The continuous-time random walk model on a graph is a Markov process where transitions have a fixed probability per unit time γ of moving to adjacent vertices, firstly introduced by Montroll and Weiss (1997). Consider a graph G with N vertices and no self-loops, this walk

can be defined by the linear differential equation that describes the probability of jumping to a connected vertex in any given time pode colocar G(V,E) e depois especificar que (i,j) é uma aresta

$$\frac{dp_i(t)}{dt} = \gamma \sum_j L_{ij} p_j(t), \tag{34}$$

where L is the Laplacian defined as $L = A - D$. A is the adjacency matrix that represents each vertex connection, given by

$$A_{ij} = \begin{cases} 1, & \text{if } (i,j) \in G \\ 0, & \text{otherwise,} \end{cases} \tag{35}$$

and D is the diagonal matrix $D_{jj} = deg(j)$ corresponding to the degree[2] of a vertex j.

In the quantum case, the nodes are quantum states that form the basis for the Hilbert space. The continuous-time quantum walk model will also be described by a differential equation, the Schrödinger equation

$$i\hbar \frac{d\,|\Psi(t)\rangle}{dt} = \hat{H}\,|\Psi(t)\rangle\,, \tag{36}$$

where $\hat{H} = -\gamma L$ is the Hamiltonian of the system. More explicitly,

$$\hat{H}_{ij} = \begin{cases} deg(j)\gamma, & \text{if } i = j; \\ -\gamma, & \text{if } i \neq j \text{ and adjacent;} \\ 0, & \text{if } i \neq j \text{ and not adjacent.} \end{cases} . \tag{37}$$

A general state of a system $|\Psi(t)\rangle$ can be written as a function of it's complex amplitudes acredito que seja contrária a relação, as amplitudes que são descritas pelo estado através da equação 28

$$q_i = \langle i|\Psi(t)|i|\Psi(t)\rangle\,, \tag{38}$$

which means 36 can be rewritten as

$$i\hbar \frac{dq_i(t)}{dt} = \sum_j \hat{H}_{ij} q_j(t). \tag{39}$$

This highlights the similarities between the Schrödinger equation and 34. One of the main differences is the complex phase i, which will result in a very different behaviour. você pode dizer que a 29 é uma quantização da 24

2 The degree of a vertex refers to the number of edges that it is connected to.

Setting $\hbar = 1$ and solving the differential equation results in the evolution operator of this walk acho que podemos ajustar, talvez a equação 32 deva subir, porque ela que é solução da equação diferencial

$$U(t) = e^{-iHt} = e^{i(-\gamma L)t} = e^{-i\gamma(A+D)t} \tag{40}$$

In the regular graph case, where D is simply the degree of the whole graph multiplied by the identity matrix, A and D will commute, meaning that the evolution operator can be written in terms of the adjacency matrix ficou muito bom isso daqui

$$U(t) = e^{-i\gamma At + i\gamma Dt} = e^{-i\gamma At} e^{i\gamma Dt} = \phi(t) e^{-i\gamma At} \tag{41}$$

since the degree matrix becomes a global phase. Applying this operator to an initial condition $\Psi(0)$, will give the state of the system at a time t

$$|\Psi(t)\rangle = U(t)\,|\Psi(0)\rangle\,. \tag{42}$$

Considering a uni-dimensional quantum system, each vertex will have at most 2 other neighboring vertices, reducing equation 37 to

$$\hat{H}_{ij} = \begin{cases} 2\gamma, & \text{if } i = j; \\ -\gamma, & \text{if } i \neq j \text{ and adjacent;} \\ 0, & \text{if } i \neq j \text{ and not adjacent.} \end{cases} \tag{43}$$

For a more detailed visualization, this quantum walk model was coded in python and figure 7 was obtained setting the transition rate to $\gamma = \frac{1}{2\sqrt{2}}$ the initial condition to $|\Psi(0)\rangle = |0\rangle$ cortou a figura

A brief look at figure 7 reveals several similarities to the coined quantum walk model of figure 6. Both have two peaks away from the origin and low probability near the origin. However, in the previous quantum walk, these characteristics were altered as a function of the chosen coin and initial condition, whereas in this case different values of γ will influence the probability distribution. For example, a lower value of γ will limit the spread of the probability distribution, as is shown in figure 9. você pode dizer que o desvio padrão é proporcional ao γ também

Moreover, the effects of altering the initial condition will also differ in the continuous-time example. For example, setting the initial condition to the balanced superposition of states $|0\rangle$ and $|1\rangle$ has no effect on the overall pattern of the probability distribution as can be seen in figure 11. Both peaks still are still present and at the same distance from the origin, with intermediate amplitudes being attenuated relative to figure 7. This behaviour is in contrast with the discrete-time case, where a change in the initial condition would dictate the number of peaks and where they would appear.

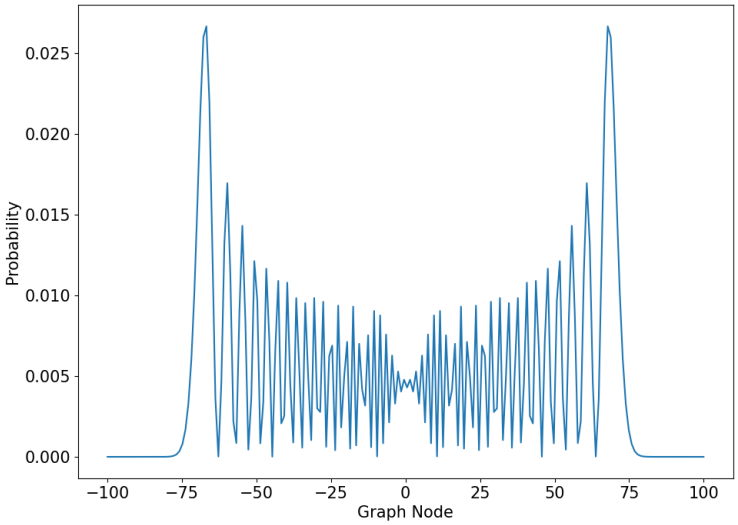

Figure 7: Probability distribution for the continuous-time quantum walk on a line, at t = 100, with initial condition $|\Psi(0)\rangle = |0\rangle$ and $\gamma = \frac{1}{2\sqrt{2}}$.

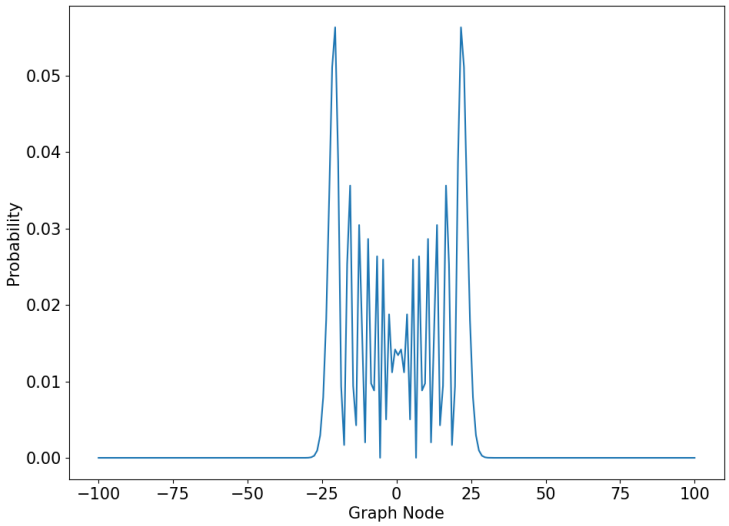

Figure 8: Probability distribution for the continuous-time quantum walk on a line, after 100 steps, with initial condition $|\Psi(0)\rangle = |0\rangle$ and $\gamma = \frac{1}{6\sqrt{2}}$.

precisa de um fechamento aqui também, alguns resultdos e referências mais talvez

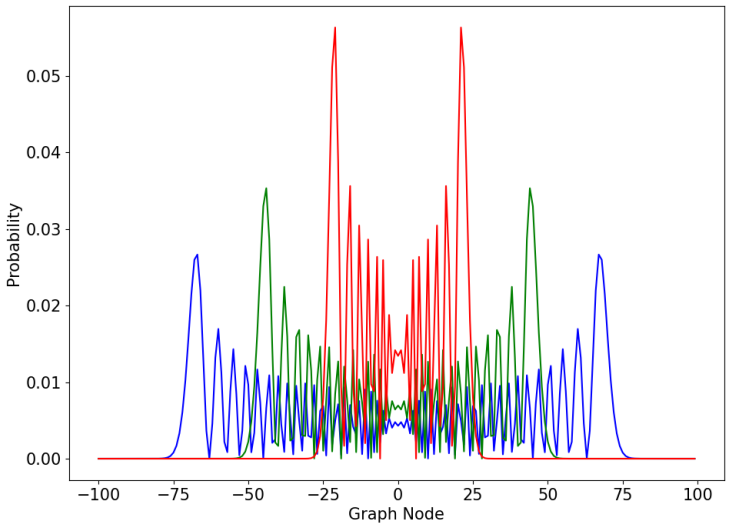

Figure 9: Temporary

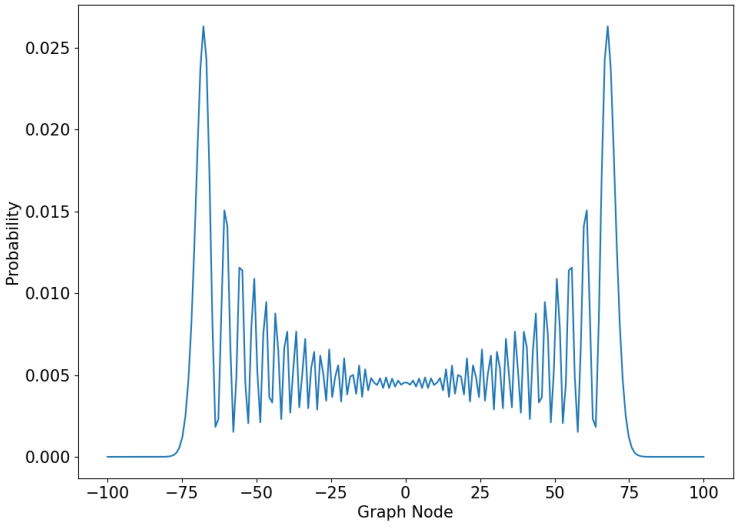

Figure 10: Probability distribution for the continuous-time quantum walk on a line, after 100 steps, with initial condition $|\Psi(0)\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ and $\gamma = \frac{1}{2\sqrt{2}}$.

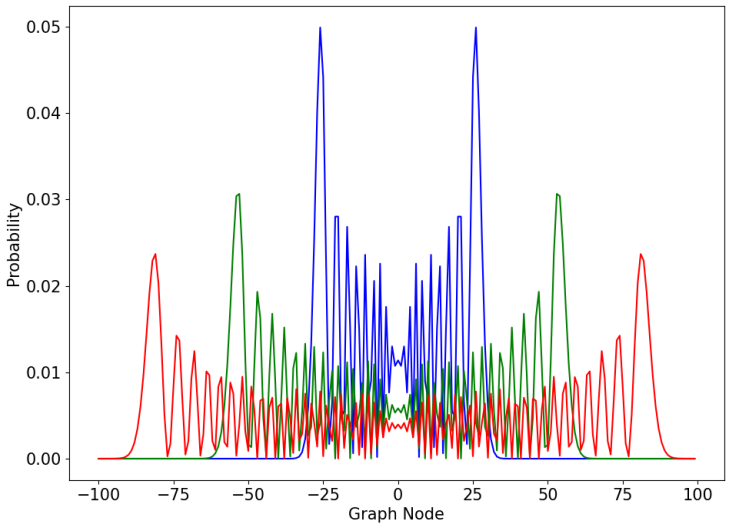

Figure 11: Temporary

3.3 STAGGERED QUANTUM WALK

Similarly to the continuous-time quantum walk, the staggered case aims to spread a transition probability to neighboring vertices but with discrete time steps. The notion of adjacency now comes from cliques[3], and the initial stage of this walk consists in partitioning the graph in several different cliques. This is called tessellation, and it is defined as the division of the set of vertices into disjoint cliques. An element of a tessellation $\mathscr{T}$ is called a polygon, and it's only valid if if all of its vertices belong to the clique in $\mathscr{T}$. The set of polygons of each tessellation must cover all vertices of the graph, and the set of tessellations ($\mathscr{T}_1$,$\mathscr{T}_2$,...,$\mathscr{T}_k$) must cover all edges.

These definitions allow the construction of operators H_1,H_2,...,H_k that will be used to propagate the probability amplitude locally, in each polygon. The state associated to each polygon is

$$\left|u_j^k\right\rangle = \frac{1}{\sqrt{|\alpha_j^k|}} \sum_{l \in \alpha_j^k} |l\rangle \tag{44}$$

where α_j^k is the $j-th$ polygon in the $k-th$ tessellation.

The unitary and Hermitian operator H_k, associated to each tessellation is defined in Portugal et al. (2017) as

$$H_k = 2\sum_{j=1}^{p} \left|u_j^k\right\rangle \left\langle u_j^k\right| - I \tag{45}$$

Solving the time-independent Schrodinger equation for this Hamiltonian gives the evolution operator

$$U = e^{i\theta_k H_k} ... e^{i\theta_2 H_2} e^{i\theta_1 H_1} \tag{46}$$

where

$$e^{i\theta_k H_k} = \cos(\theta_k) I + i \sin(\theta_k) H_k \tag{47}$$

since $H_k^2 = I$.trocar and por since. Posso referir livro do nielsen

The simplest use case of this quantum walk model is the one-dimensional lattice, where the minimum tessalations are

$$\mathscr{T}_\alpha = \{\{2x, 2x+1\} : x \in Z\} \tag{48}$$

$$\mathscr{T}_\beta = \{\{2x+1, 2x+2\} : x \in Z\} \tag{49}$$

3 A clique is defined as the subset of vertices of an undirected graph such that every two distinct vertices in each clique are adjacent.

Each element of the tessellation has a corresponding state, and the uniform superposition of these states is

$$|\alpha_x\rangle = \frac{|2x\rangle + |2x+1\rangle}{\sqrt{2}} \tag{50}$$

$$|\beta_x\rangle = \frac{|2x+1\rangle + |2x+2\rangle}{\sqrt{2}} \tag{51}$$

One can now define Hamiltonians H_α and H_β as trocar operators por hamiltonians, talvez

$$H_\alpha = 2\sum_{x=-\infty}^{+\infty} |\alpha_x\rangle\langle\alpha_x| - I \tag{52}$$

$$H_\beta = 2\sum_{x=-\infty}^{+\infty} |\beta_x\rangle\langle\beta_x| - I \tag{53}$$

The Hamiltonian evolution operator reduces to

$$U = e^{i\theta H_\beta} e^{i\theta H_\alpha} \tag{54}$$

and applying it to an initial condition $|\Psi(0)\rangle$ results in the time evolution operator

$$U|\Psi(t)\rangle = U^t|\Psi(0)\rangle \tag{55}$$

Having defined the time evolution operator, the walk is ready to be coded with a certain initial condition and θ value, to better understand how the probability distribution spreads through time. você pode acrescentar que o θ terá um papel similar ao γ no controle do desvio-padrão

For the first case study, the initial condition will be a uniform superposition of states $|0\rangle$ and $|1\rangle$ and the θ value will be varied in order to understand how this parameter impacts the walk

The overall structure of the probability distribution remains the same, the difference is that the walker is more likely to be found further away from the origin as the angle increases.

Another interesting case study is to see how the initial condition affects the dynamics of the system

Similarly to the coined case, each initial condition results in asymmetric probability distributions, $|\Psi(0)\rangle = |0\rangle$ leads to a peak in the left-hand side while condition $|\Psi(0)\rangle = |1\rangle$ results in a peak in the right-hand side. As was shown in 12, the uniform superposition of both these conditions results in a symmetric probability distribution. acho que você pode explicar um pouco mais o papel de θ através dos gráficos e podemos pensar se fazemos gráficos do desvio-padrão para este e o contínuo

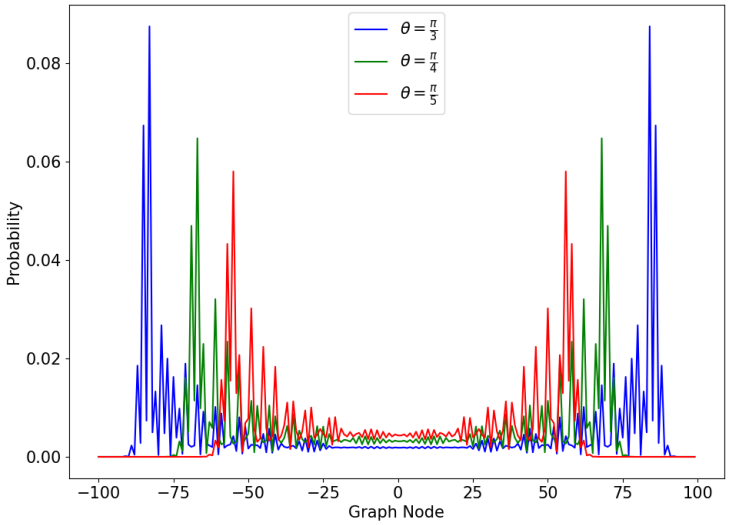

Figure 12: Probability distribution for the staggered quantum walk on a line after 50 steps, with initial condition $|\Psi(0)\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$, for multiple angles.

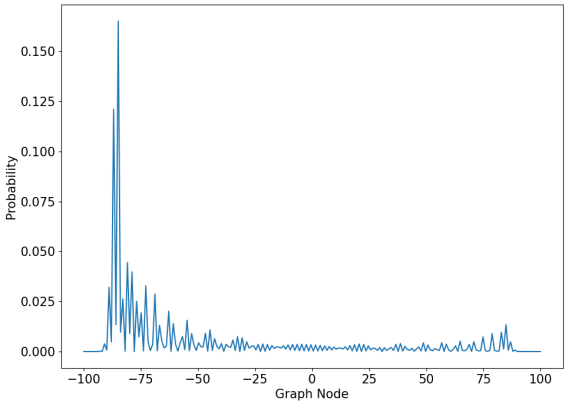

Figure 13: $|\Psi(0)\rangle = |0\rangle$

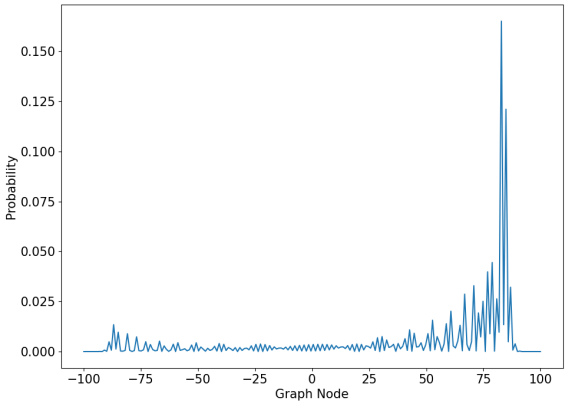

Figure 14: $|\Psi(0)\rangle = |1\rangle$

3.4 Search problems with Quantum Walks

In classical computation, a *spatial search problem* focuses on finding marked points in a finite region of space. Defining this region with graphs is fairly straightforward, the vertices of the graph are the search space, and the edges define what transitions are possible through the search space. As was previously mentioned in 2.1, exhaustively searching through an unstructured space, by means of a classical random walk for example, would mean that in the worst case, one would have to take as many steps to find the marked points as there

are vertices in the graph. Quantum computing provides an alternative to this complexity through Grover's algorithm, and applying some of his ideas to the coined quantum walk not only allows a quantum counterpart to the random walk search, but also further insight into the algorithm itself.

acho que você precisa delimitar o que fará ao longo desta seção, dizer que tratará os três modelos e a busca

3.4.1 *Coined*

Following Portugal (2018)'s definition, a good first step is to borrow the diffusion from Grover's algorithm and invert the sign of the state corresponding to the marked vertex while leaving unmarked vertices unchanged. This is done through the following operator eu trocaria a notação de $\mathcal{F}$ por $\mathcal{O}$ e dizer que é um oráculo

$$\mathcal{F}' = I - 2\sum_{x\in M} |x\rangle \langle x| \tag{56}$$

where M is the set of marked vertices and $\mathcal{F}'$ is an analogue to Grover's oracle. For one marked vertex, this oracle can be written as você pode até dizer que $M = \{0\}$

$$\mathcal{F}' = I - 2\,|0\rangle \langle 0| \tag{57}$$

Notice that there is no loss of generality by choosing the marked vertex as 0, since the labelling of the vertices is arbitrary.

The next step is to combine the evolution operator from the coined quantum walk model with the oracle

$$U' = U\mathcal{F}' \tag{58}$$

Similarly to the simple coined case, the walker starts at $|\Psi(0)\rangle$ and evolves following the rules of an unitary operator U followed by the sign inversion of marked vertices. The walker's state after an arbitrary number of steps will be

$$\Psi(t) = (U')^t\,|\Psi(0)\rangle\,. \tag{59}$$

For a better understanding of the search problem in the coined quantum walk model, consider a graph where all the vertices are connected and each vertex has a loop that allows transitions to itself, as shown in figure **??**. não precisa dizer que são arcos também The next step is to label the arcs using notation $\{(v, v'), v \geqslant 0 \wedge v' \leqslant N-1\}$ where N is the total

number of vertices and (v, v') are the position and coin value, respectively, in the coined model. The shift operator, now called flip-flop shift operator, is

$$S\left|v1\right\rangle\left|v2\right\rangle = \left|v2\right\rangle\left|v1\right\rangle. \tag{60}$$

The coin operator is defined as

$$C = I_N \otimes G \tag{61}$$

where prefiro s a D

$$G = 2\left|D\right\rangle\left\langle D\right| - I \tag{62}$$

is the Grover coin with $\left|D\right\rangle$ being the diagonal state of the coin space. Given both of these operators, the evolution is defined for the unmarked case similarly to 24

$$U = S(I \otimes G). \tag{63}$$

Marking an element in a complete graph is done through the following oracle

$$\mathcal{F}'' = \mathcal{F}' \otimes I = (I_N - 2\left|0\right\rangle\left\langle 0\right|) \otimes I_N = I_{N^2} - 2\sum_v \left|0\right\rangle\left|v\right\rangle\left\langle 0\right|\left\langle v\right|, \tag{64}$$

that can be seen, in the arc notation, as an operator that marks all arcs leaving 0.

Recalling 58, the modified evolution operator can be written as

$$U' = S(I \otimes G)\mathcal{F}'' = S(I \otimes G)\mathcal{F}' \otimes I = S(\mathcal{F}' \otimes G), \tag{65}$$

and the state of the system will evolve according to equation 59.

As was shown in Portugal (2018), maximum probability of the marked vertex is achieved after $\frac{\pi}{2}\sqrt{N}$ steps. Figure 15 is the result of coding and plotting the evolution of this probability distribution, for graphs of varying sizes. It shows that the probability is close to one at *approximately* the predicted ideal steps, because of the discrete nature of the walk. The probability distributions have a stair-like shape, because transitions in this model only occur on even numbered time steps, because of how the unmodified evolution operator was constructed.

3.4.2 *Staggered*

The process for defining the search problem in this model is similar to the coined quantum walk case. The oracle still inverts the sign of a certain state and amplifies it, and the system's state will still be described by equation 59. However,instead of using a coin, the staggered model takes advantage of the notions of cliques and tessellations, as was shown in chapter

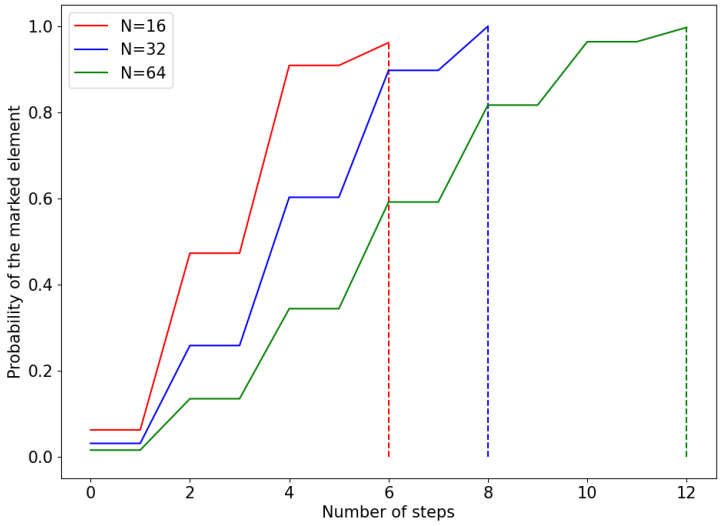

Figure 15: Discrete-time coined quantum walk search for a complete graph with 16, 32 and 64 nodes.

3.3, which means the unmodified evolution operator has to be defined for an undirected complete graph.

As was shown in figure **??**, the vertices in a complete graph are all neighbors. This is a special case because this is the only connected graph where the tessellation cover can be done by one tessellation, since the graph is it's own clique. The minimum tessellations required to cover this structures are defined by the one clique that encompasses all N nodes of the graph

$$\mathscr{T}_\alpha = \{\{0, 1, 2, ..., N-1\}\}. \tag{66}$$

The associated polygon can then be described as the balanced superposition of all the nodes in the graph

$$|\alpha\rangle = \frac{1}{\sqrt{N}} \sum_{v=0}^{N-1} |v\rangle \,. \tag{67}$$

The Hamiltonian, as defined in 45, is falta índice no somatório

$$H_\alpha = 2 \sum_{0}^{1} |\alpha\rangle \langle\alpha| - I = 2 |\alpha_0\rangle \langle\alpha_0| - I \tag{68}$$

The unmodified evolution operator from equation 46

$$U = e^{i\theta_k H_k} ... e^{i\theta_2 H_2} e^{i\theta_1 H_1} \tag{69}$$

reduces to the single Hamiltonian case

$$U = e^{i\theta H_\alpha}. \tag{70}$$

The choice of the θ value is an important one, since maximum probability is achieved at $\theta = \frac{\pi}{2}$, as shown in figure 16. Since $H_\alpha^2 = I$, equation 70 can be rewritten as

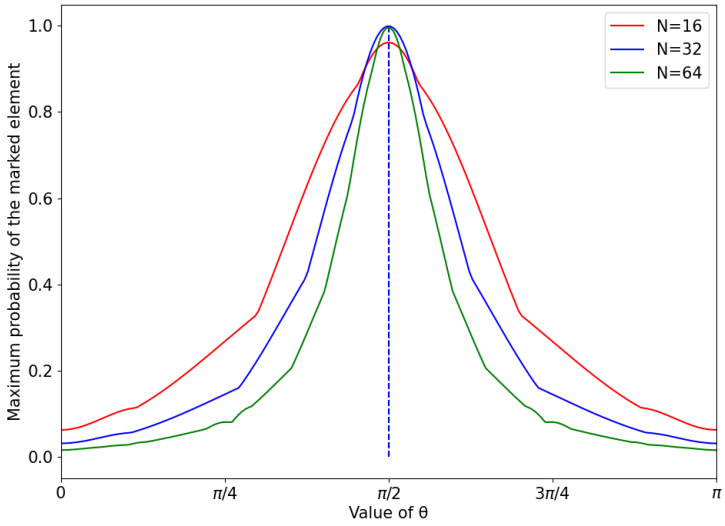

Figure 16: Maximum probability of the marked element as a function of the θ value plotted from 0 to π for number of nodes $N = 64, 128$ and 256.

$$U = e^{-i\frac{\pi}{2}H_\alpha} = \cos\frac{\pi}{2}I + i\sin\frac{\pi}{2}H_\alpha = iH_\alpha = i(2\left|\alpha_0\right\rangle\left\langle\alpha_0\right| - I). \tag{71}$$

Having defined the the evolution operator associated with the complete graph, the next step is to use the oracle

$$\mathcal{F}' = I_N - 2\left|0\right\rangle\left\langle 0\right|, \tag{72}$$

to create the modified evolution operator associated with the search

$$U' = U\mathcal{F}'. \tag{73}$$

The walk achieves the same result as Grover's algorithm after $\frac{\pi}{4}\sqrt{N}$ steps, as shown in figure 17. This plot also shows that the probabilities converge to 1 as N increases, this is because time is discretized and deviations to the ideal steps will matter less for bigger values of N.

precisa de um fechamento também aqui

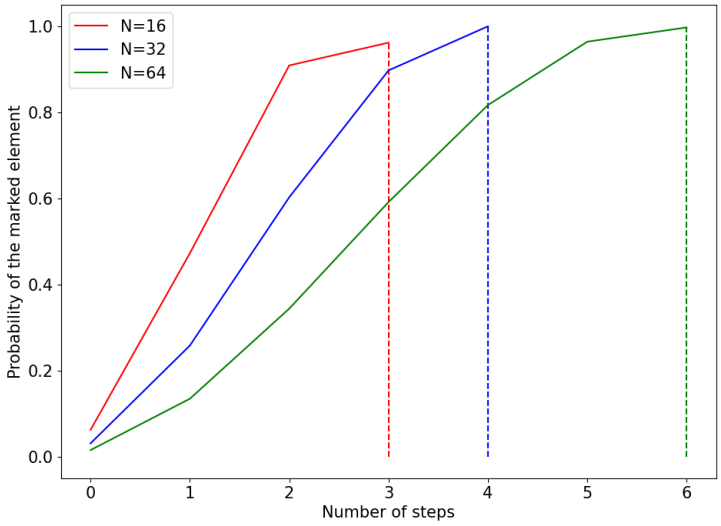

Figure 17: Staggered quantum walk search for a complete graph with 16, 32 and 64 nodes.

3.4.3 *Continuous*

As was previously seen, the continuous-time quantum walk model is defined by an evolution operator obtained by solving Schrödinger's equation

$$U(t) = e^{-iHt}. \tag{74}$$

The search problem requires introducing an oracle to the Hamiltonian, that will mark an arbitrary vertex m

$$H' = -\gamma L - |m\rangle \langle m|. \tag{75}$$

Since the complete graph is a regular graph, the operator can be rewritten in terms of the adjacency matrix plus the marked element. Considering $|0\rangle$ is marked,

$$U'(t) = e^{iH't} = e^{i(-\gamma L - |0\rangle\langle 0|)t} = e^{i(-\gamma A + \gamma D - |0\rangle\langle 0|)t} = e^{-i\gamma(A+|0\rangle\langle 0|)t + i\gamma Dt}. \tag{76}$$

The degree matrix is again $D = dI$, which means it will commute with $A + |0\rangle \langle 0|$ and become a global phase

$$U'(t) = e^{-i\gamma(A+|0\rangle\langle 0|)t} e^{i\gamma Dt} = \phi(t) e^{-i\gamma(A+|0\rangle\langle 0|)t}. \tag{77}$$

As was show by Zalka (1999), the value of γ is crucial for the success of the search. As γ increases, the contribution of the marked element in the Hamiltonian decreases, and as γ

approaches 0 the contribution of the adjacency matrix decreases. To find the optimum value, the Hamiltonian can be rewritten by adding multiples of the identity matrix to the adjacency matrix H′ é uma notação ruim, confunde com derivada e acredito não ser necessário aqui

$$H' = -\gamma(A + NI) - |0\rangle\langle 0| = -\gamma N |s\rangle\langle s| - |0\rangle\langle 0| \tag{78}$$

where $|s\rangle = \frac{1}{\sqrt{N}}\sum_i |i\rangle$. Now it is obvious that, for $\gamma = \frac{1}{N}$, the Hamiltonian is $H = -|s\rangle\langle s| - |0\rangle\langle 0|$. It's eigenstates are proportional to $|s\rangle \pm |w\rangle$ and eigenvalues are $-1 - \frac{1}{\sqrt{N}}$ and $-1 + \frac{1}{\sqrt{N}}$, respectively. This means that the evolution rotates from the state of balanced superposition to the marked vertex state in time $\frac{\pi}{\Delta E} = \frac{\pi}{2}\sqrt{N}$ which is, as was shown by Zalka (1999), optimal and equivalent to Grover's algorithm. Plotting ΔE as a function of γN, as can be seen in figure 18, has a minimum at $\gamma N = 1$. The difference between the largest eigenvalue and second largest, plotted in the y-axis, is the smallest for a value of $\gamma N = 1 \implies \gamma = \frac{1}{N}$, which will correspond to the maximum probability for the marked vertex, in optimal steps.

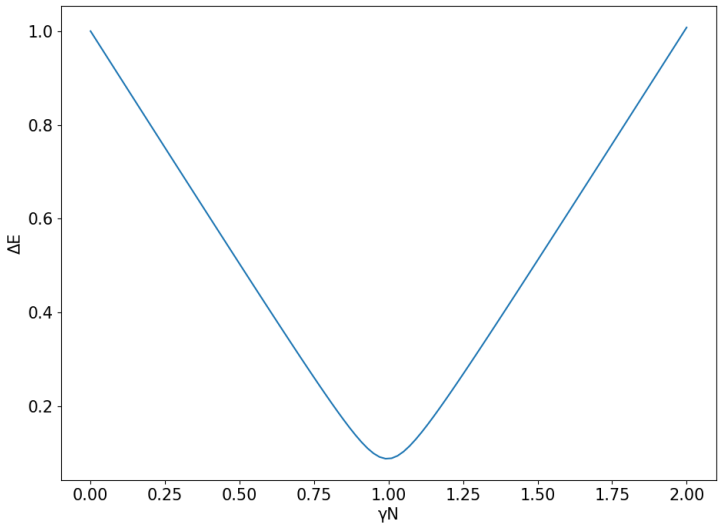

Figure 18: Value of the difference between the largest eigenvalue and the second largest, plotted as a function of γN, for $N = 512$.

Figure 19 shows the evolution of the probability of the marked vertex in time, which is continuous in this model. In contrast with previous models, the distributions are smooth and reach exactly one, since the walk is allowed to evolve to exactly the ideal time steps.

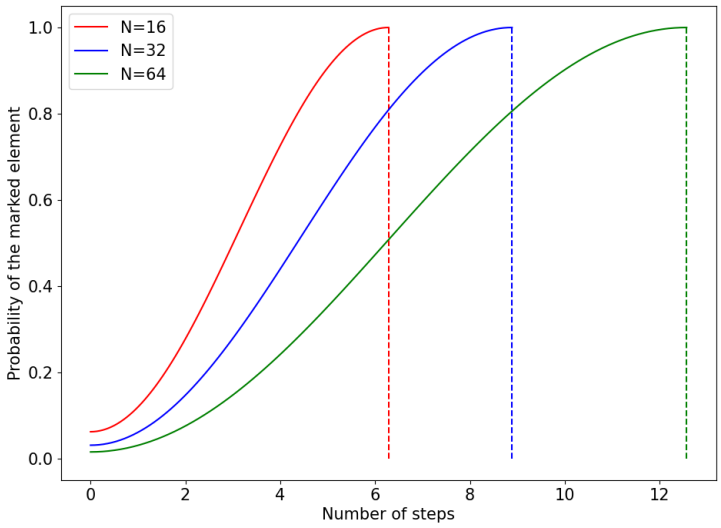

Figure 19: Continuous quantum walk search for a complete graph with 16, 32 and 64 vertices.

4

IMPLEMENTATIONS AND APPLICATIONS

4.0.1 *Continuous*

4.0.2 *Staggered*

5

DISCUSSIONS AND CONCLUSION

5.1 CONCLUSIONS

5.2 PROSPECT FOR FUTURE WORK

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SUPPORT MATERIAL