Grover Algorithms

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Let's take a quantum state

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$$\alpha_x \in R, \quad \alpha_x \geq 0, \quad 0 \leq x < N.$$

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We want to measure the k-th state. In 1996 Lov Grover proposed an idea that is quite obvious, simple, but really ingenious.

Before performing the measurement, it is necessary to modify the coefficients of the state vector so that the coefficient corresponding to the required state becomes substantially the largest $|\alpha_k|^2 \approx 1$.

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In this lecture, we will show that even in the case of quantum computing the most important work is to create efficient algorithms and justify them.

The implementation of quantum algorithms is also an important stage and this can be done efficiently using, for example, Qiskit tool. This topic will be covered in the next lecture.

Quantum search algorithm

- We have a list of values of arguments x of function f:

$$X = \{0, 1, \ldots, 2^n - 1\}.$$

Let's denote $N = 2^n$.

We need to find some $x \in X_1 \subset X$ such that $f(x) = 1$

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- The complexity of any search algorithm in non-ordered sets is $\mathcal{O}(N)$.

Let us consider the case of an oracle, which is so important in cryptography.

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Let us say that in 10 seconds we can check 2^{25} key variants (this is a fairly accurate estimate of the computing power of modern personal computers).

Then checking all variants of the key will take 10×2^{31} seconds, so more than 700 years.

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Then finding the key will require only 2^{28} cycles of the algorithm and it will take only 80 seconds.

Quantum operator for the calculation of oracle function f

Suppose we know the classical algorithm for computing f.

Let's recall how we then construct a quantum computing operator for this function

$$U_f(x, \phi): \quad |x, \phi\rangle \quad \rightarrow \quad |x, \phi \oplus f(x)\rangle\,,$$

where $|x, f(x)\rangle = |x\rangle \otimes |f(x)\rangle$,

and $|\phi\rangle$ is our chosen extra qubit.

A general scheme of the Grover algorithm.

- Generate a superposition of all n qubits in a Hilbert vector space.

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We chose the auxiliary qubit $|\phi\rangle = |0\rangle$, this is not our final choice, but it will help to understand the search algorithm more easily.

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But if we now perform the measurement, we will know the value of $f(x)$ at one randomly selected point only and we will lose information about the values of $f(x)$ at all other points

Preparing for the measurement operation

We have a quantum state

$$|\psi\rangle = \sum_{x=0}^{N-1} \alpha_x |x\rangle ,$$

$$\alpha_x \in R, \quad \alpha_x \geq 0, \quad 0 \leq x < N.$$

We change the signs of the amplitudes:

$$\alpha_x = \begin{cases} \alpha_x, & \text{if } f(x) = 0, \\ -\alpha_x, & \text{if } f(x) = 1. \end{cases}$$

Let us denote the quantum operator performing such an operation by

$$Z_f : \quad |x\rangle \quad \rightarrow \quad (-1)^{f(x)} |x\rangle .$$

Perform an inversion transformation with respect to the mean value

1. Calculate the average

$$A = \frac{1}{N} \sum_{x=0}^{N-1} \alpha_x$$

2. Perform the transformation

$$\alpha_x := 2A - \alpha_x, \quad x = 0, \ldots, N-1.$$

As an example, let's consider the execution of the first iteration of Grover's algorithm.

Suppse, that $f(x_k) = 1$, and at all other points $f(x_j) = 0$.

Also assume that at the initial moment all coefficients are positive $\alpha_x > 0$ and equal.

After the first iteration we get $\alpha_k \approx 3\alpha_x$.

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After the first iteration we get $\alpha_k \approx 3\alpha_x$.

After the second iteration the coefficient α_k is increased even more with respect to the other coefficients

$$\alpha_k \approx 5\alpha_x, \quad x \neq k.$$

After completion $\frac{\pi}{8}\sqrt{N}$ iterations

$$\alpha_k^2 \approx \sum_{j \neq k} \alpha_j^2.$$

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Let's consider the example: $n = 6$, $N = 64$. Then we get the following probabilities that we will measure the required qubit

$$\begin{aligned}
\text{it} = 0 \quad & p = 0.015625, \\
\text{it} = 1 \quad & p = 0.134827, \\
\text{it} = 2 \quad & p = 0.343895, \\
\text{it} = 3 \quad & p = 0.59138, \\
\text{it} = 6 \quad & p = 0.996586, \\
\text{it} = 12 \quad & p = 7.05e-05.
\end{aligned}$$

After t iterations of Grover's algorithm, we measure the value of the last qubit.

- If we get a unit value, then we have a Hilbert subspace

$$\frac{1}{\sqrt{2^k}} \sum_{i=1}^{k} |x_i, 1\rangle .$$

Next we simply measure the remaining qubits and obtain one of the sought solutions $x_i \in X_1$.

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- If we measure the last qubit and get a zero value, then calulations we must be repeated.

It is clear that it is not sufficient to know details of the algorithm, but also it is important to know why this algorithm so efficiently solve the given problem.

Therefore next we will perform a more complete mathematical analysis explaining how this algorithm works.

One important question remains not answered – how to choose the optimal number of iterations in the general case, when more than one "marked" state may exist.

Good news that the mathematics here is not complicated,

Sign-change transformation

We present a universal and efficient way how to perform this transformation.

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Let's take the following control qubit:

$$|\phi\rangle = H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

it will be used to calculate the oracle operator

Let X_0 denote the set of states $x \in X$, where $f(x) = 0$, and X_1 denote the set, where $f(x) = 1$.

Let's calculate the image of the function

$$U_f(|\psi,\phi\rangle) = \sum_{x=0}^{N-1} \alpha_x U_f |x,\phi\rangle = \sum_{x\in X_0} \alpha_x U_f |x,\phi\rangle + \sum_{x\in X_1} \alpha_x U_f |x,\phi\rangle$$

$$= \frac{1}{\sqrt{2}}\Big(\sum_{x\in X_0} \alpha_x |x, 0\oplus 0\rangle - \sum_{x\in X_0} \alpha_x |x, 1\oplus 0\rangle + \sum_{x\in X_1} \alpha_x |x, 0\oplus 1\rangle$$

$$- \sum_{x\in X_1} \alpha_x |x, 1\oplus 1\rangle \Big) = \sum_{x\in X_0} \alpha_x |x,\phi\rangle + \sum_{x\in X_1} (-\alpha_x) |x,\phi\rangle .$$

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By using the operator Z_f, we can write this result in a compact form:

$$Z_f |\psi\rangle = \sum_{x\in X_0} \alpha_x |x\rangle - \sum_{x\in X_1} \alpha_x |x\rangle .$$

Inversion transformation

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$$D: \quad \sum_{x=0}^{N-1} \alpha_x |x\rangle \quad \rightarrow \quad \sum_{x=0}^{N-1} (2A - \alpha_x) |x\rangle ,$$

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This is done by the operator (for now it is just a mathematical definition)

$$\mathcal{D} = \begin{pmatrix} 2/N-1 & 2/N & \cdots & 2/N \\ 2/N & 2/N-1 & \cdots & 2/N \\ \cdots & \cdots & \cdots & \cdots \\ 2/N & 2/N & \cdots & 2/N-1 \end{pmatrix} .$$

It is easy to verify that matrix $\mathcal{D}$ is unitary:

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We also define another similar operator, which also changes the signs of the amplitudes of the quantum ground states

$$Z_{OR}: \quad |x\rangle \rightarrow \begin{cases} |x\rangle, & x = 0^n, \\ -|x\rangle, & x \neq 0^n. \end{cases}$$

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The transformation D can be implemented as follows

$$D = H^{\otimes n} \, Z_{OR} \, H^{\otimes n}, \quad n = \log N.$$

Then we write Grover's operator G as follows:

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Let's define two independent superpositions of quantum states

$$|\psi_0\rangle = \frac{1}{\sqrt{|X_0|}} \sum_{x \in X_0} |x\rangle , \quad |\psi_1\rangle = \frac{1}{\sqrt{|X_1|}} \sum_{x \in X_1} |x\rangle .$$

Then we get the linear combination of the two vector structures:

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle = \sqrt{\frac{|X_0|}{N}}\, |\psi_0\rangle + \sqrt{\frac{|X_1|}{N}}\, |\psi_1\rangle \,.$$

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It is easy to see that

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It is easy to see that

$$Z_f |\psi_0\rangle = |\psi_0\rangle , \quad Z_f |\psi_1\rangle = - |\psi_1\rangle .$$

We can also express the operator Z_{OR} as follows

$$Z_{OR} = 2 |0^n\rangle \langle 0^n| - I.$$

Then we can write the transformation with respect to the mean value:

$$H^{\otimes n} Z_{OR} H^{\otimes n} = 2 |\psi\rangle \langle \psi| - I,$$

and Grovers's transformation

$$G = \left(2\left|\psi\right\rangle\left\langle\psi\right| - I\right) Z_f.$$

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After performing simple algebraic calculations, we get

$$G\left|\psi_0\right\rangle = \frac{|X_0| - |X_1|}{N}\left|\psi_0\right\rangle + \frac{2\sqrt{|X_0| \cdot |X_1|}}{N}\left|\psi_1\right\rangle,$$

$$G\left|\psi_1\right\rangle = -\frac{2\sqrt{|X_0| \cdot |X_1|}}{N}\left|\psi_0\right\rangle + \frac{|X_0| - |X_1|}{N}\left|\psi_1\right\rangle.$$

The 2×2 matrix $\mathcal{M}$ corresponding to this operator is defined as follows

$$\mathcal{M} = \begin{pmatrix} \frac{|X_0|-|X_1|}{N} & -\frac{2\sqrt{|X_0|\cdot|X_1|}}{N} \\ \frac{2\sqrt{|X_0|\cdot|X_1|}}{N} & \frac{|X_0|-|X_1|}{N} \end{pmatrix}.$$

The geometric interpretation of quantum unitary transformations can be based on analysis of turns in space, this is also the case for $\mathcal{M}$:

$$\mathcal{M} = \begin{pmatrix} \sqrt{\frac{|X_0|}{N}} & -\sqrt{\frac{|X_1|}{N}} \\ \sqrt{\frac{|X_1|}{N}} & \sqrt{\frac{|X_0|}{N}} \end{pmatrix}^2 = \begin{pmatrix} \cos(2\theta) & -\sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{pmatrix},$$

where

$$\theta = \sin^{-1}\left(\sqrt{|X_1/|N}\right).$$

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where

$$\theta = \sin^{-1}\left(\sqrt{|X_1/|N}\right).$$

We have the following initial state:

$$|\psi\rangle = \cos(\theta)\,|\psi_0\rangle + \sin(\theta)\,|\psi_1\rangle\,.$$

Then one Grover's iteration rotates this vector by an angle (2θ):

$$G\,|\psi\rangle = \cos(3\theta)\,|\psi_0\rangle + \sin(3\theta)\,|\psi_1\rangle\,.$$

After two iterations we obtain the quantum state

$$G^2 |\psi\rangle = \cos(5\theta) |\psi_0\rangle + \sin(5\theta) |\psi_1\rangle ,$$

and after t iterations:

$$G^t |\psi\rangle = \cos((2t+1)\theta) |\psi_0\rangle + \sin((2t+1)\theta) |\psi_1\rangle .$$

If we have a quantum state

$$|\psi\rangle = \alpha |\psi_0\rangle + \beta |\psi_1\rangle = \frac{\alpha}{\sqrt{|X_0|}} \sum_{x \in X_0} |x\rangle + \frac{\beta}{\sqrt{|X_1|}} \sum_{x \in X_1} |x\rangle$$

then the probability of measuring any state $x \in X_1$ is equal to $|\beta|^2$.

By definition, the probability of measuring some specific state $x \in X_1$ is equal to $|\beta|^2/|X_1|$ and the number of such states $|X_1|$.

Grover's approximation after t iterations is defined as follows:

$$G^t |\psi\rangle = \cos((2t+1)\theta) |\psi_0\rangle + \sin((2t+1)\theta) |\psi_1\rangle$$

so the probability of measuring any state $x \in X_1$ is equal to

$$\sin^2 ((2t+1)\theta).$$

In order to maximize this probability and minimize the number of iterations, it is necessary to take the number of iterations (a natural number) that is closest to

$$(2t+1)\theta = \frac{\pi}{2} \quad \rightarrow \quad t = \frac{\pi}{4\theta} - \frac{1}{2} \quad \rightarrow \quad t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor.$$

If we have only one element in the set X_1, then

$$\theta = \sin^{-1}\left(\sqrt{1/N}\right) \approx \sqrt{1/N} \quad \rightarrow \quad t \approx \frac{\pi}{4}\sqrt{N}.$$

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If we have s possible solutions, then

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What strategy can be recommended for choosing the number of iterations t, if we do not have information about s ?