

Lecture 5:

Unstructured search and Grover's algorithm

Luís Soares Barbosa
www.di.uminho.pt/~lsb/



Universidade do Minho



INESC TEC



INTERNATIONAL IBERIAN
NANOTECHNOLOGY
LABORATORY



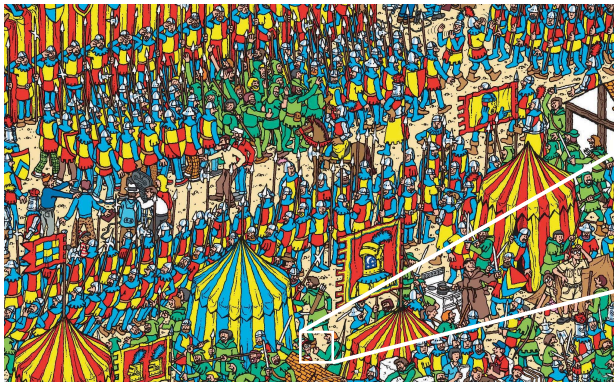
**UNU
EGOV**

Quantum Computation

Mestrado em Engenharia Física

Universidade do Minho, 2026-27

Unstructured search



Unstructured search

Search problem

- **Search space:** unstructured / unsorted
- **Asset:** a tool to efficiently **recognise** a solution

Example: Searching in a sorted vs unsorted database

- find a name in a telephone directory
- find a phone number in a telephone directory

Unstructured search

Note that a procedure to **recognise** a solution does **not** need to rely on a previous knowledge of it.

Example: password recognition

- $f(x) = 1$ iff $x = 123456789$ (f **knows** the password)
- $f(x) = 1$ iff $\text{hash}(x) = \text{c9b93f3f0682250b6cf8331b7ee68fd8}$
(f **recognises** a correct password, but does not know it as inverting a hash function is, in general, very hard.)

Unstructured search

A typical formulation

Given a function $f : 2^n \rightarrow 2$ such that there exists a **unique** number, encoded by a binary string w , st

$$f(x) = \begin{cases} 1 & \Leftarrow x = w \\ 0 & \Leftarrow x \neq w, \end{cases}$$

determine w .

A classical solution

- 0 evaluations of f : probability of success: $\frac{1}{2^n}$
- 1 evaluation of f : probability of success: $\frac{2}{2^n}$
(choose a solution at random; if test fails choose another)
- 2 evaluations of f : probability of success: $\frac{3}{2^n}$.
- k evaluations of f : probability of success: $\frac{k+1}{2^n}$.

A quantum algorithm

Grover's algorithm (1996): A quadratic speed up

- Worst case for a classic algorithm: 2^n evaluations of f
- Worst case for Grover's algorithm: $\sqrt{2^n}$ evaluations of f

where n is the number of qubits necessary to represent the input (i.e. the search space)

(Variants of) this algorithm can be applied in a **multitude of scenarios**:

- Searching through unstructured databases
- Finding passwords
- Route planning
- Solving SAT problems (and **NP**-problems in general)

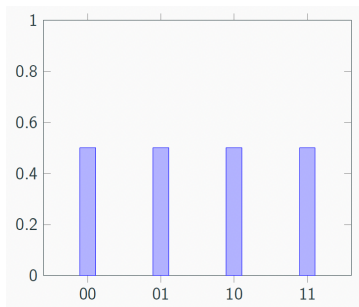
Key Ideas

The algorithm resorts to two quantum resources:

1. **superposition**
2. **interference**
(to decrease amplitude of wrong answers and increase amplitude of the right ones)

Key Ideas: Superposition

Suppose $f : \{0, 1\}^2 \rightarrow \{0, 1\}$ with $f(\textcolor{red}{1}0) = 1$



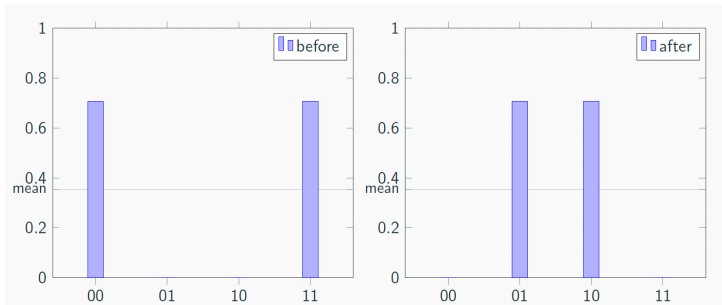
$$\frac{1}{2}(|00\rangle + |01\rangle + \textcolor{red}{|10\rangle} + |11\rangle)$$

Key Ideas: Interference

Act on **amplitudes** through the following map:

$$x \mapsto \text{mean} + (\text{mean} - x)$$

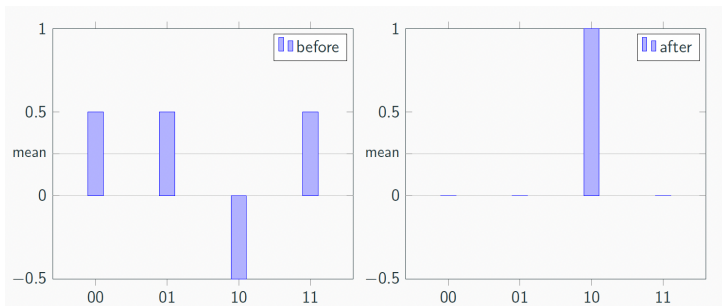
(inversion about the mean)



Intuitively mass of some states was given to others

Key Ideas: Interference

See the effect when the right amplitude has an opposite phase:



Intuitively, mass of wrong answers was given to the right one.

The strategy

1. Put all **possible answers** in **uniform superposition**
2. **Label** the **right answer** by **flipping** its phase
3. **Amplify** the amplitude of the **right answer** (through inversion about the mean)
4. **Iterate** through steps 2 and 3 until one can be sure to measure the **right answer** with high probability

Step 1: Label the solution

Let $N = 2^n$, then search space

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle$$

can be expressed in terms of two states separating the **solution** state and **the rest**:

$$|w\rangle \text{ and } |r\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \in N, x \neq w} |x\rangle$$

which forms a basis for a 2-dimensional subspace of the original N -dimensional space. Thus,

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle = \underbrace{\frac{1}{\sqrt{N}} |w\rangle}_{\text{solution}} + \underbrace{\sqrt{\frac{N-1}{N}} |r\rangle}_{\text{the rest}}$$

Step 1: Label the solution

As discussed in a previous lecture, an **oracle** for f 'kicks back' the relevant phase:

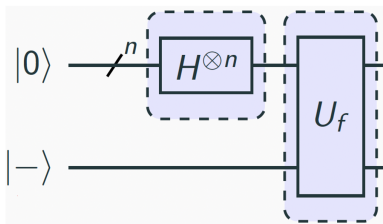
$$U_f|x\rangle|-\rangle = (-1)^{f(x)}|x\rangle|-\rangle$$

In particular, if w is the **solution**, then its phase is flipped (because $f(x) = 1$)

$$U_f|w\rangle|-\rangle = -|w\rangle|-\rangle$$

Step 1: Label the solution

Summing up, this circuit



encodes the following quantum state in the top qubits:

$$\sum_{x \neq w} |x\rangle\langle x| - |w\rangle\langle w| = I - 2|w\rangle\langle w|$$

The **solution** is identified but an observer is unable to retrieve it because the square of the amplitudes for any basis state is always $\frac{1}{N}$.

Step 2: Boost the right amplitude

The oracle performs a phase shift over an **unknown** state, marking the solution but not changing the probability of retrieving it.

Thus, one needs a mechanism to **boost the probability of retrieving the solution**, which will be accomplished by another phase shift, but now applied to well-known vectors.

Consider, the following program

$$P = 2|0\rangle\langle 0| - I$$

Can you see its effect?

Step 2: Boost the right amplitude

P flips basis states different from $|0\rangle$, i.e. applies a -1 phase shift to all vectors in the subspace orthogonal to $|0\rangle$, i.e. spanned by all the basis states $|x\rangle$, for $x \neq 0$:

$$\begin{aligned} P &= 2|0\rangle\langle 0| - I \\ &= |0\rangle\langle 0| + (-1)(I - |0\rangle\langle 0|) \\ &= |0\rangle\langle 0| + (-1) \sum_{x \neq 0} |x\rangle\langle x| \end{aligned}$$

Thus, $P|x\rangle = -(-1)^{\delta_{x,0}}|x\rangle$

Step 2: Boost the right amplitude

Then, use P to define an operator

$$W = H^{\otimes n} P H^{\otimes n}$$

A simple calculation yields,

$$\begin{aligned} W &= H^{\otimes n} P H^{\otimes n} \\ &= H^{\otimes n} (2|0\rangle\langle 0| - I) H^{\otimes n} \\ &= 2(H^{\otimes n}|0\rangle\langle 0|H^{\otimes n}) - H^{\otimes n} I H^{\otimes n} \\ &= 2|\psi\rangle\langle\psi| - I \end{aligned}$$

denoting $H^{\otimes n}|0\rangle$ by $|\psi\rangle$.

Operator W boosts the probability of finding the right solution.

Can you see why?

Step 2: Boost the right amplitude

First note that

$$|\psi\rangle\langle\psi| = \frac{1}{N} \sum_{x,y \in N} |x\rangle\langle y|$$

because

$$\begin{aligned} |\psi\rangle\langle\psi| &= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle \frac{1}{\sqrt{N}} \sum_{y=0}^{N-1} \langle y| \\ &= \frac{1}{N} \sum_{x=0}^{N-1} |x\rangle \sum_{y=0}^{N-1} \langle y| \\ &= \frac{1}{N} \sum_{x,y \in N} |x\rangle\langle y| \end{aligned}$$

The effect of W : to *invert about the average*

$$\begin{aligned}
 W \left(\sum_k \alpha_k |k\rangle \right) &= (2|\psi\rangle\langle\psi| - I) \sum_k \alpha_k |k\rangle \\
 &= \left(2 \left(\frac{1}{N} \sum_{x,y \in N} |x\rangle\langle y| \right) - I \right) \sum_k \alpha_k |k\rangle \\
 &= 2 \left(\frac{1}{N} \sum_{x,y,k \in N} \alpha_k |x\rangle\langle y|k\rangle \right) - \sum_k \alpha_k |k\rangle \\
 &= 2 \left(\underbrace{\frac{1}{N} \sum_{k \in N} \alpha_k}_{\alpha \text{ (mean)}} \sum_{x \in N} |x\rangle \right) - \sum_{k \in N} \alpha_k |k\rangle \\
 &= 2 \alpha \sum_{k \in N} |k\rangle - \sum_{k \in N} \alpha_k |k\rangle \\
 &= \sum_{k \in N} (2\alpha - \alpha_k) |k\rangle
 \end{aligned}$$

The effect of W : to *invert about the average*

The effect of W is to transform the amplitude of each state so that it is as far above the average as it was below the average prior to its application, and vice-versa:

$$\alpha_k \mapsto 2\alpha - \alpha_k$$

W boosts the “right” amplitude; slightly reduces the others.

Example: $N = 2^2 = 4$, $w = 01$

The algorithm starts with a uniform superposition

$$H^{\otimes 2}|0\rangle = \frac{1}{2} \sum_{k=0}^3 |k\rangle$$

which the **oracle** turns into

$$\frac{1}{2}|00\rangle - \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle$$

The effect of **inversion about the average** is

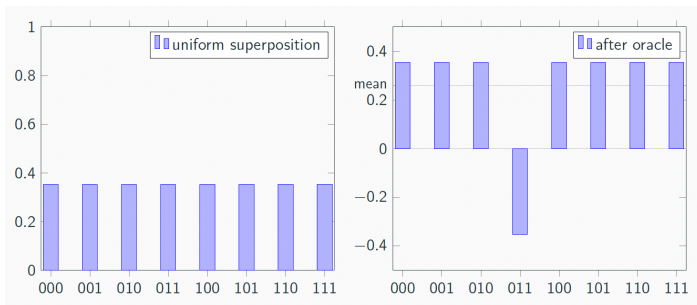
$$2 \underbrace{\alpha \sum_k |k\rangle}_{\begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix}} - \underbrace{\sum_k \alpha_k |k\rangle}_{\begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}} = \begin{bmatrix} \frac{2}{4} - \frac{1}{2} \\ \frac{2}{4} + \frac{1}{2} \\ \frac{2}{4} - \frac{1}{2} \\ \frac{2}{4} - \frac{1}{2} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Measuring returns the solution with probability 1

Example: $N = 2^3 = 8$, $w = 011$

Starting point: all amplitudes $\alpha_k = \frac{1}{2\sqrt{2}}$

After the oracle: $\alpha_{011} = -\frac{1}{2\sqrt{2}}$; all the others remain.



Example: $N = 2^3 = 8$, $w = 011$

After the boost:

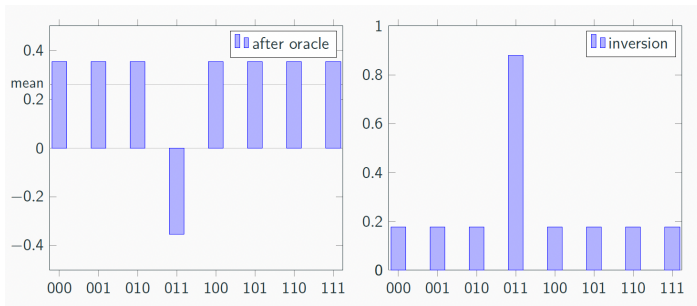
$$\begin{aligned}
 & (2|\psi\rangle\langle\psi| - I) \left(|\psi\rangle - \frac{2}{2\sqrt{2}}|011\rangle \right) \\
 &= 2|\psi\rangle\langle\psi|\psi\rangle - |\psi\rangle - \frac{2}{\sqrt{2}}|\psi\rangle\langle\psi|011\rangle + \frac{1}{\sqrt{2}}|011\rangle \\
 &= 2|\psi\rangle\langle\psi|\psi\rangle - |\psi\rangle - \frac{2}{\sqrt{2}}\frac{1}{2\sqrt{2}}|\psi\rangle + \frac{1}{\sqrt{2}}|011\rangle \\
 &= |\psi\rangle - \frac{1}{2}|\psi\rangle + \frac{1}{\sqrt{2}}|011\rangle \\
 &= \frac{1}{2}|\psi\rangle + \frac{1}{\sqrt{2}}|011\rangle
 \end{aligned}$$

As $|\psi\rangle = \frac{1}{2\sqrt{2}} \sum_{k=0}^7 |k\rangle$, we end up with

$$\frac{1}{2} \left(\frac{1}{2\sqrt{2}} \sum_{k=0}^7 |k\rangle \right) + \frac{1}{\sqrt{2}}|011\rangle = \frac{1}{4\sqrt{2}} \sum_{k=0, k \neq 3}^7 |k\rangle + \frac{5}{4\sqrt{2}}|011\rangle$$

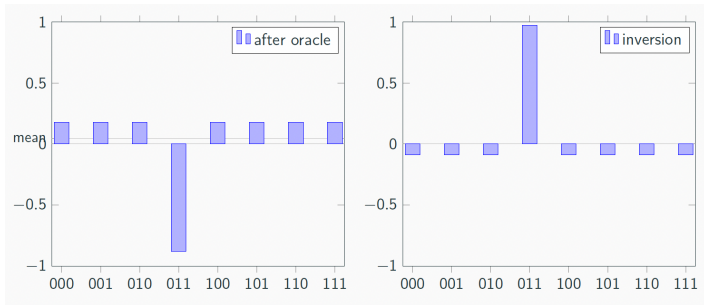
Example: $N = 2^3 = 8$, $w = 011$

In pictures:



Example: $N = 2^3 = 8$, $w = 011$

Making a second iteration yields



with

- $\alpha_{011} = \frac{11}{8\sqrt{2}}$
- all remaining amplitudes: $\frac{-1}{8\sqrt{2}}$

Example: $N = 2^3 = 8$, $w = 011$

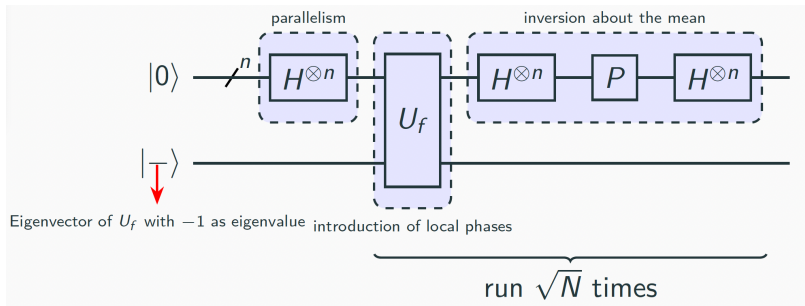
The probability of measuring the state corresponding to the solution is

$$\left| \frac{11}{8\sqrt{2}} \right|^2 = \frac{121}{128} \approx 94,5\%$$

Thus,

Grover's is an **iterative** algorithm

Grover algorithm : The iterator $G = WU_f$



Question

How many iterations are needed?

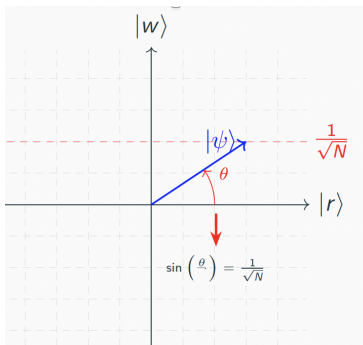
What's behind the scenes?

- The key is the selective shifting of the phase of one state of a quantum system, one that satisfies some condition, at each iteration.
- Performing a phase shift of π is equivalent to multiplying the amplitude of that state by -1 : the amplitude for that state changes, but the probability of being in that state remains the same
- Subsequent transformations take advantage of that difference in amplitude to single out that state and increase the associated probability.
- This would **not be possible if the amplitudes were probabilities**, not holding extra information regarding the phase of the state in addition to the probability — it's a **quantum feature**.

A geometric perspective on G

Initial state: $|\psi\rangle = \frac{1}{\sqrt{N}}|w\rangle + \sqrt{\frac{N-1}{N}}|r\rangle$

$|w\rangle$ and $|r\rangle$ form an orthonormal basis for a 2-dimensional vector space in which one may analyse Grover's algorithm.



A geometric perspective on G

Another basis is given by $|\psi\rangle$ and the state **orthogonal** to $|\psi\rangle$:

$$|\bar{\psi}\rangle = \sqrt{\frac{N-1}{N}}|w\rangle - \frac{1}{\sqrt{N}}|r\rangle$$

Define an angle θ st $\sin \theta = \frac{1}{\sqrt{N}}$ (and, of course, $\cos \theta = \sqrt{\frac{N-1}{N}}$), and express both bases as

$$\begin{aligned} |\psi\rangle &= \sin \theta |w\rangle + \cos \theta |r\rangle & |\bar{\psi}\rangle &= \cos \theta |w\rangle - \sin \theta |r\rangle \\ |w\rangle &= \sin \theta |\psi\rangle + \cos \theta |\bar{\psi}\rangle & |r\rangle &= \cos \theta |\psi\rangle - \sin \theta |\bar{\psi}\rangle \end{aligned}$$

A geometric perspective on G

G has two components:

- **Oracle** V which applies a phase shift to $|w\rangle$: **reflection over $|r\rangle$** .
Actually, $V = 2|r\rangle\langle r| - I$ (or, equivalently, $I - 2|w\rangle\langle w|$). Thus,

$$V(\alpha_w|w\rangle + \alpha_r|r\rangle) = -\alpha_w|w\rangle + \alpha_r|r\rangle$$

- **Amplifier** $W = 2|\psi\rangle\langle\psi| - I$ which applies a phase shift to all vectors in the subspace orthogonal to $|\psi\rangle$: **reflection over $|\psi\rangle$** .

A geometric perspective on G

Exercise.

Now, express the action of V in the basis $|\psi\rangle, |\bar{\psi}\rangle$ to perform afterward the second reflection.

$$\begin{aligned} V|\psi\rangle &= -\sin\theta|w\rangle + \cos\theta|r\rangle \\ &= -\sin\theta(\sin\theta|\psi\rangle + \cos\theta|\bar{\psi}\rangle) + \cos\theta(\cos\theta|\psi\rangle - \sin\theta|\bar{\psi}\rangle) \\ &= -\sin^2\theta|\psi\rangle - \sin\theta\cos\theta|\bar{\psi}\rangle + \cos^2\theta|\psi\rangle - \cos\theta\sin\theta|\bar{\psi}\rangle \\ &= (-\sin^2\theta + \cos^2\theta)|\psi\rangle - 2\sin\theta\cos\theta|\bar{\psi}\rangle \\ &= \cos 2\theta|\psi\rangle - \sin 2\theta|\bar{\psi}\rangle \end{aligned}$$

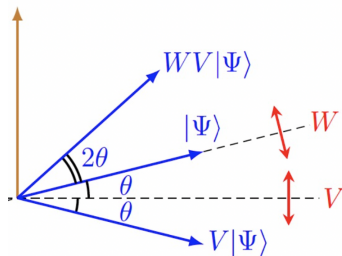
(Recall the little riddle on base changing to date your loved one ...)

A geometric perspective on G

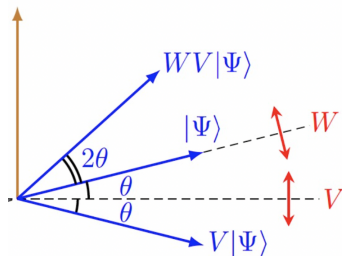
Then, the second reflection over $|\psi\rangle$ yields the effect of the Grover iterator:

$$G|\psi\rangle = WV|\psi\rangle = \cos 2\theta|\psi\rangle + \sin 2\theta|\bar{\psi}\rangle$$

which boils down to a 2θ rotation:



How many times should G be applied?



From this picture, we may also conclude that the **angular distance to cover** towards an amplitude maximizing the probability of finding the correct solution is

$$\frac{\pi}{2} - \theta = \frac{\pi}{2} - \arcsin\left(\frac{1}{\sqrt{N}}\right)$$

How many times should G be applied?

Thus, the ideal number of iterations is

$$t = \left\lceil \frac{\frac{\pi}{2} - \arcsin \frac{1}{\sqrt{N}}}{2\theta} \right\rceil$$

where $|x|$ denotes the integer closest to x .

A lower bound for θ gives an upper bound for t
— for N large $\theta \approx \sin \theta = \frac{1}{\sqrt{N}}$. Thus,

$$t = \frac{\frac{\pi\sqrt{N}-2}{2\sqrt{N}}}{\frac{2}{\sqrt{N}}} \approx \frac{\pi}{4}\sqrt{N}$$

Complexity

So, G applied t times leaves the system within an angle θ of $|w\rangle$. Then, a measurement in the computational basis yields the correct solution with probability

$$|\langle w | G^t | \psi \rangle|^2 \geq \cos^2 \theta = 1 - \sin^2 \theta = \frac{N-1}{N}$$

which, for large N , is very close to 1.

On the other hand,
Execution time wrt (classical) exhaustive search:

from $\mathcal{O}(N)$ to $\mathcal{O}(\sqrt{N})$