Lecture 21

# Grover search algorithm (extended with Qiskit examples)

*of the course "Fundamentals of Quantum Computing"*
*(by IAPS and QUANTERALL)*

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# Plan



Essence

Words as point in Hilbert space

Steps of the Grover search algorithm

Grover algorithm on a two-qubit system

Qiskit notebook

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Lov Kumar Grover

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The objects (haystack) must be represented as points in a Hilber space. The vectors of the objects which we try to find span a subspace in this space.

The Grover algorithm constructs operators that transform a given initial state into a state which has a maximal component in the subspace of desired objects (*amplitude amplification*).

**Definition 6.22** Let S denote the set of objects we are searching for, and let $m \geq 1$ be the cardinality of this set. The set S is called solution set, and we call its elements solutions. For the algorithm to search an $x \in \mathrm{S} \subset \{0,\ldots,N-1\}$, where $N = 2^n$, we define the input and output register as $\mathbb{H}^{I/O} = \P\mathbb{H}^{\otimes n}$. Furthermore, we denote the set of objects that are not a solution by

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and define the subspaces

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and the operators

$$P_{\mathrm{S}} := \sum_{x \in \mathrm{S}} |x\rangle\langle x|$$

$$P_{\mathrm{S}^{\perp}} := \sum_{x \in \mathrm{S}^{\perp}} |x\rangle\langle x| = \mathbf{1}^{\otimes n} - P_{\mathrm{S}}$$

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$$|\Psi_{\mathrm{S}}\rangle := \frac{1}{\sqrt{m}} \sum_{x \in \mathrm{S}} |x\rangle$$

$$|\Psi_{\mathrm{S}^{\perp}}\rangle := \frac{1}{\sqrt{N-m}} \sum_{x \in \mathrm{S}^{\perp}} |x\rangle$$

Every state $|\Psi\rangle \in H^{I/O}$ can be decomposed as:

$$|\Psi\rangle = \left(P_{S^\perp} + P_S\right)|\Psi\rangle = \sum_{x \in S^\perp} \Psi_x |x\rangle + \sum_{x \in S} \Psi_x |x\rangle$$

Remember, measuring the state $|\Psi\rangle$ means:

**Definition 5.35** Let $n \in \mathbb{N}$ and for $j \in \{0, \ldots, n-1\}$ and $\alpha \in \{0, \ldots, 3\}$ (or, equivalently, $\alpha \in \{0, x, y, z\}$) define

$$\Sigma_\alpha^j := \mathbf{1}^{\otimes n-1-j} \otimes \sigma_\alpha \otimes \mathbf{1}^{\otimes j} \quad \in \mathrm{B}_{\mathrm{sa}}\left({}^{\P}\mathbb{H}^{\otimes n}\right),$$

where the $\sigma_\alpha$ are as in Definition 2.21. The **observation of a state in the quantum register** ${}^{\P}\mathbb{H}^{\otimes n}$ is defined as the measurement of all compatible observables

$$\Sigma_z^j = \mathbf{1}^{\otimes n-1-j} \otimes \sigma_z \otimes \mathbf{1}^{\otimes j}$$

for $j \in \{0, \ldots, n-1\}$ in the state of the quantum register. Such an observation is also called **read-out** or **measurement** of the register.

The goal of the algorithm to create states $|\Psi\rangle$ for which the probability to observe an $x \in S$ is maximized. This is accomplished by starting from an initial state $|\Psi_0\rangle$ and by applying suitable transformations which increase the component in $H_S$.

$$\mathbf{P}\left\{\begin{array}{l}\text{Observation of } |\Psi\rangle \text{ projects} \\ \text{onto a state } |x\rangle \text{ with } x \in \mathrm{S}\end{array}\right\} \underbrace{=}_{(2.62)} \left|\left|P_{\mathrm{S}}|\Psi\rangle\right|\right|^2 \underbrace{=}_{(6.137)} \left|\left|\sum_{x\in\mathrm{S}} \Psi_x |x\rangle\right|\right|^2$$

$$\underbrace{=}_{(2.14)} \sum_{x\in\mathrm{S}} |\Psi_x|^2 \,.$$

# Decision if a state is a solution

$$g : \{0,\dots,N-1\} \longrightarrow \{0,1\}$$
$$x \longmapsto g(x) := \begin{cases} 0 & \text{if } x \in S^{\perp} \\ 1 & \text{if } x \in S \end{cases}$$

$$\widehat{U}_g\left(|x\rangle \otimes |y\rangle\right) := |x\rangle \otimes |y \boxplus g(x)\rangle$$

where $|y\rangle$ belongs to an auxiliary register $H^W$.

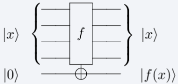
Reminder

$$|a \boxplus b\rangle := \bigotimes_{j=m-1}^{0} |a_j \overset{2}{\oplus} b_j\rangle$$

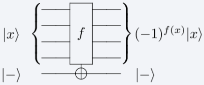
$$u \overset{2}{\oplus} v := (u+v) \mod 2$$

▼ Circuit Construction of a Grover Oracle (click to expand)

If we have our classical function $f(x)$, we can convert it to a reversible circuit of the form:




If we initialise the 'output' qubit in the state $|-\rangle$, the phase kickback effect turns this into a Grover oracle (similar to the workings of the Deutsch-Jozsa oracle):




We then ignore the auxiliary ($|-\rangle$) qubit.

**Lemma 6.24** *For the oracle $U_g$ and the state*

$$|\omega_i\rangle = |\omega_f\rangle = |-\rangle := \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

*in the auxiliary register $\mathbb{H}^W$ one has for arbitrary $|\Psi\rangle \in \mathbb{H}^{I/O}$*

$$\widehat{U}_g\left(|\Psi\rangle \otimes |-\rangle\right) = \left(R_{S^\perp}|\Psi\rangle\right) \otimes |-\rangle\,,$$

*where*

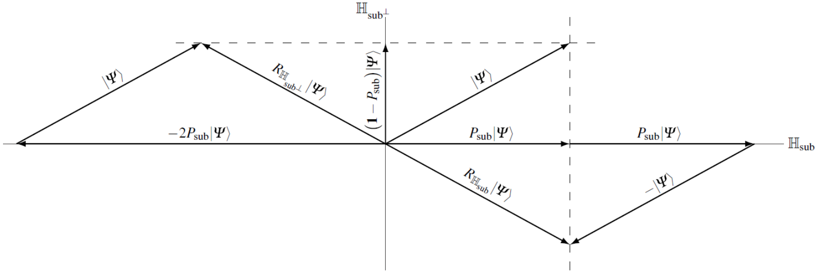
$$\begin{aligned} R_{S^\perp}|\Psi\rangle &= \sum_{x\in S^\perp} \Psi_x|x\rangle - \sum_{x\in S} \Psi_x|x\rangle \\ &= (\mathbf{1}^{\otimes n} - 2P_S)|\Psi\rangle\,. \end{aligned}$$

$R_{S\perp}$ can be viewed as reflection about $H_{S\perp}$:

**Definition 6.25** Let $\mathbb{H}_{\text{sub}}$ be a subspace of the HILBERT space $\mathbb{H}$, and let $P_{\text{sub}}$ be the projection onto this subspace. The **reflection about the subspace** $\mathbb{H}_{\text{sub}}$ is defined as the operator

$$R_{\text{sub}} := 2P_{\text{sub}} - \mathbf{1}\,. \tag{6.147}$$

If the subspace is one-dimensional and spanned by a $|\Psi\rangle \in \mathbb{H}$, we simply write $R_\Psi$ and call this a reflection about $|\Psi\rangle$.



$\mathbb{H}_{\text{sub}^\perp}$
$|\Psi\rangle$
$R_{\mathbb{H}_{\text{sub}^\perp}}|\Psi\rangle$
$(\mathbf{1}-P_{\text{sub}})|\Psi\rangle$
$|\Psi\rangle$
$-2P_{\text{sub}}|\Psi\rangle$
$P_{\text{sub}}|\Psi\rangle$
$P_{\text{sub}}|\Psi\rangle$
$\mathbb{H}_{\text{sub}}$
$R_{\mathbb{H}_{\text{sub}}}|\Psi\rangle$
$-|\Psi\rangle$

**Definition 6.26** Let S be the solution set with cardinality $m \geq 1$. For the algorithm to search for an $x \in \mathrm{S} \subset \{0, \ldots, N-1\}$, where $N = 2^n$, we define the initial state in the input/output register as

$$|\Psi_0\rangle := \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle \in \mathbb{H}^{I/O}. \tag{6.148}$$

Moreover, we define the angle

$$\theta_0 := \arcsin\left(\sqrt{\frac{m}{N}}\right) \in \left[0, \frac{\pi}{2}\right], \tag{6.149}$$

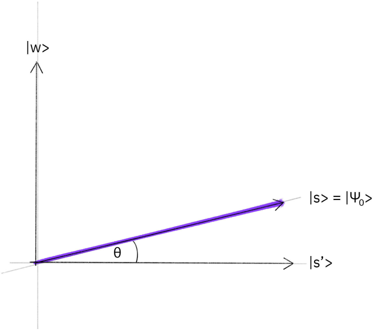
and with the help of $|\Psi_0\rangle$ we define the operator

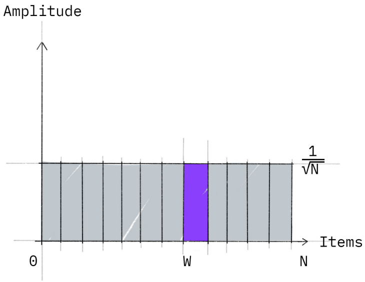
$$R_{\Psi_0} = 2|\Psi_0\rangle\langle\Psi_0| - \mathbf{1}^{\otimes n} \tag{6.150}$$

on $\mathbb{H}^{I/O}$ as well as the initial state in the composite system

$$|\widehat{\Psi}_0\rangle := |\Psi_0\rangle \otimes |-\rangle \in \mathbb{H}^{I/O} \otimes \mathbb{H}^W. \tag{6.151}$$

$$|\Psi_0\rangle = \cos\theta_0 |\Psi_{\mathrm{S}^\perp}\rangle + \sin\theta_0 |\Psi_{\mathrm{S}}\rangle$$




$$|s'\rangle \equiv |\Psi_{S\perp}\rangle, \ |w\rangle \equiv |\Psi_S\rangle$$

**Definition 6.27** The **GROVER iteration** is defined as the operator

$$\widehat{G} := \left(R_{\Psi_0} \otimes \mathbf{1}\right) \widehat{U}_g$$

on $\mathbb{H}^{I/O} \otimes \mathbb{H}^W$.

As we will now show, the GROVER iteration $G$ transforms separable states in $\mathbb{H}^{I/O} \otimes \mathbb{H}^W$ of the form $|\widehat{\Psi}_j\rangle = |\Psi_j\rangle \otimes |-\rangle$ to separable states $|\widehat{\Psi}_{j+1}\rangle = |\Psi_{j+1}\rangle \otimes |-\rangle$ of a similar form. We will see that in the input/output register $\mathbb{H}^{I/O}$ an application of $\widehat{G}$ can then be viewed as *a rotation of* $2\theta_0$ *in* $\mathbb{H}^{I/O}$ *in the direction of* $|\Psi_S\rangle$.

**Proposition 6.28** *For $j \in \mathbb{N}_0$ let*

$$|\widehat{\Psi}_j\rangle := \widehat{G}^j |\widehat{\Psi}_0\rangle .$$

*Then we have for all $j \in \mathbb{N}_0$*

$$|\widehat{\Psi}_j\rangle = |\Psi_j\rangle \otimes |-\rangle$$

*with $|\Psi_j\rangle \in \mathbb{H}^{I/O}$ and*

$$|\Psi_j\rangle = \cos\theta_j |\Psi_{S^\perp}\rangle + \sin\theta_j |\Psi_S\rangle ,$$

*where*

$$\theta_j = (2j+1)\theta_0 .$$

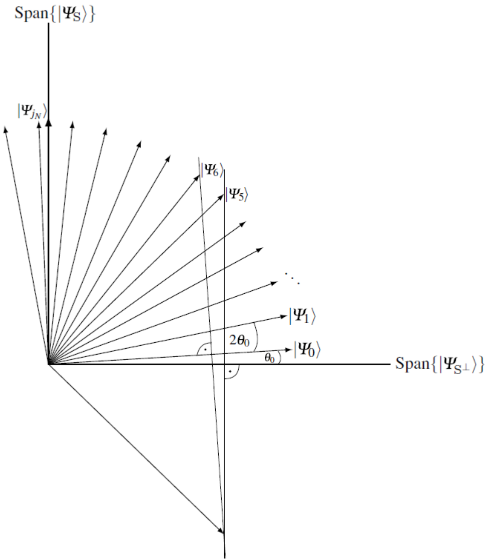
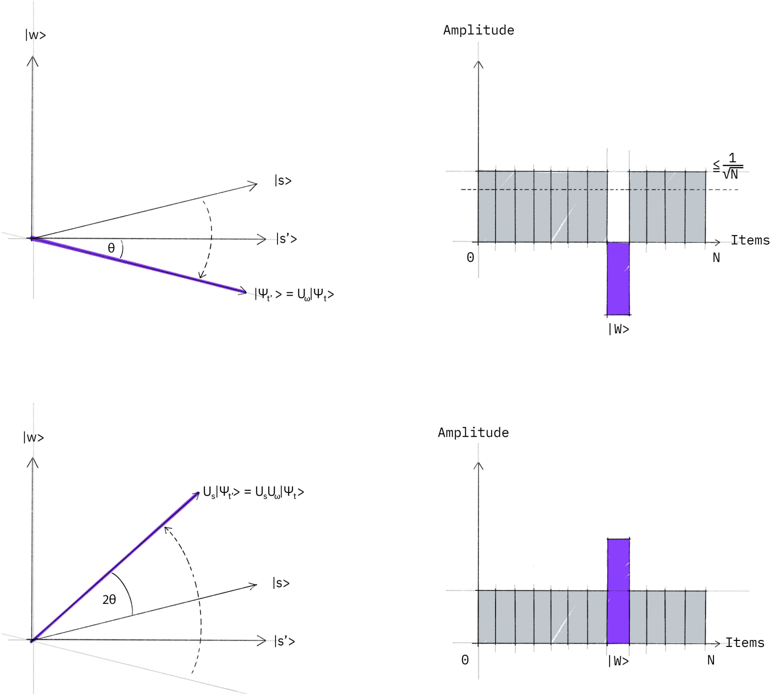



**Fig. 6.6** Geometry of the GROVER iteration in the input/output register with $m = 5, N = 2^{10}$ and $j_N = 11$. In the two-dimensional subspace $\mathrm{Span}\{|\Psi_{S^\perp}\rangle, |\Psi_S\rangle\}$ the initial state $|\Psi_0\rangle$ is rotated towards $|\Psi_S\rangle$. The illustrated transition from $|\Psi_5\rangle$ to $|\Psi_6\rangle$ shows that $\widehat{G}$ in the sub-system $I/O$ first performs a reflection about $|\Psi_{S^\perp}\rangle$ and then a reflection about $|\Psi_0\rangle$. The vector immediately to the right of $|\Psi_{j_N}\rangle$ is $|\Psi_S\rangle$ and is a state in the subspace $\mathbb{H}_S$ of the solution set. We can see that $|\Psi_{j_N}\rangle$ comes close to that



|w>
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≤ 1/√N
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|s>
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Amplitude
Items
0
|W>
N

$$\mathbf{P}\left\{\begin{array}{l}\text{Observation of } |\Psi_j\rangle \text{ projects} \\ \text{onto a state } |x\rangle \text{ with } x \in \mathrm{S}\end{array}\right\} = \big|\big|P_{\mathrm{S}}|\Psi_j\rangle\big|\big|^2 \underbrace{=}_{(6.137),(6.138),\,(6.154)} \sin^2\theta_j$$

**Lemma 6.29** *Let* S *be the solution set with cardinality* $m \geq 1$, *and let* $N = 2^n$ *be the number of objects in which we search for solutions. If we apply the* GROVER *iteration* $\widehat{G}$

$$j_N := \left\lfloor \frac{\pi}{4\arcsin\left(\sqrt{\frac{m}{N}}\right)} \right\rfloor \tag{6.158}$$

*times to* $|\widehat{\Psi}_0\rangle$ *and observe the state* $|\Psi_{j_N}\rangle$ *in the input/output register, then the probability to observe in the sub-system* $\mathbb{H}^{I/O}$ *a state* $|x\rangle$ *with* $x \in \mathrm{S}$ *satisfies*

$$\mathbf{P}\left\{\begin{array}{l}\textit{Observation of } |\Psi_j\rangle \textit{ projects} \\ \textit{onto a state } |x\rangle \textit{ with } x \in \mathrm{S}\end{array}\right\} \geq 1 - \frac{m}{N}\,. \tag{6.159}$$

# Steps of the Grover search algorithm

**Input**: A set $\{0,\dots,N-1\}$ of $N = 2^n$ objects that contains a subset $\mathrm{S}$ of $m \geq 1$ objects to be searched for and an oracle-function $g : \{0,\dots,N-1\} \rightarrow \{0,1\}$ that takes the value 1 in $\mathrm{S}$ and the value 0 elsewhere

**Step 1**: In $\mathbb{H}^{I/O} \otimes \mathbb{H}^{W} = \P\mathbb{H}^{\otimes n} \otimes \P\mathbb{H}$ prepare the composite system in the state $|\widehat{\Psi}_0\rangle = |\Psi_0\rangle \otimes |-\rangle$ with

$$|\Psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle\,.$$

The number of computational steps required for Step 1 scales for $N \rightarrow \infty$ with

$$S_{\textsc{Grover}1}(N) \in O(1)$$

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The number of computational steps required for Step 1 scales for $N \rightarrow \infty$ with

$$S_{\mathrm{GROVER1}}(N) \in O(1)$$

**Step 2**: With $\theta_0 = \arcsin\left(\sqrt{\frac{m}{N}}\right)$ apply the transform $\widehat{G} = (R_{\Psi_0} \otimes \mathbf{1})\widehat{U}_g$

$$j_N = \left\lfloor \frac{\pi}{4\theta_0} \right\rfloor$$

times to $|\widehat{\Psi}_0\rangle$ in order to transform the composite system to the state

$$|\widehat{\Psi}_{j_N}\rangle = \widehat{G}^{j_N} |\widehat{\Psi}_0\rangle .$$

The number of computational steps required for Step 2 scales for $N \rightarrow \infty$ with

$$S_{\mathrm{GROVER2}}(N) \in O\left(\sqrt{\frac{N}{m}}\right)$$

**Step 3**: Observe the sub-system $\mathbb{H}^{I/O}$ and infer from the observed state $|x\rangle$ the value $x \in \{0,\ldots,N-1\}$. The number of computational steps required for Step 3 scales for $N \to \infty$ with

$$S_{\text{GROVER3}}(N) \in O(1)$$

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**Step 4**: By evaluating $g(x)$, check if $x \in \mathrm{S}$. The number of computational steps required for Step 4 scales for $N \to \infty$ with

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**Step 4**: By evaluating $g(x)$, check if $x \in \mathrm{S}$. The number of computational steps required for Step 4 scales for $N \rightarrow \infty$ with

**Output**: A solution $x \in \mathrm{S}$ with probability no less than $1 - \frac{m}{N}$

# Grover algorithm on a two-qubit system

in this case Eq. 6.149 becomes

$$\theta_0 = \arcsin(\sqrt{1/4}) = \pi/6$$

$j_N$ for the equation 6.158 is

$$j_N = \left[\frac{\pi}{4\arcsin(\sqrt{1/4})}\right] = 1$$

Then the Grover transformation $G^{j_N} \equiv G^1$ yields
$\theta_{j_N} = (2j_N + 1)\theta_0 = \pi/2$ , i.e.
$G^{j_N}|\Psi_0\rangle = \cos\theta_{j_N}|\Psi_{S_\perp}\rangle + \sin\theta_{j_N}|\Psi_S\rangle \equiv |\Psi_S\rangle$
For the case when $S \equiv |11\rangle$ see the notebook linked in the following slide.

Qiskit notebook

https://qiskit.org/textbook/ch-algorithms/grover.html

NEXT LECTURE

NOVEMBER 25, 2022

THANK YOU FOR YOUR ATTENTION!

БЛАГОДАРЯ ЗА ВНИМАНИЕТО!