# Indian Institute of Science, Bengaluru

Grover's search implementation on a database


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## 1 The genius of Grover's algorithm ...

Before we see the actual implementation of Grover's search in a quantum circuit, it is worthwhile to get a high-level glimpse of the intuitions that led to the development of this 'optimal' algorithm.

Lov Grover thought of the search problem as an **evolution of a system from an initial uniform superposition state to a target state**, under the action of a Hamiltonian comprising potential energy and kinetic energy. A highly negative potential energy at the target state that would gravitate the system towards it. Whereas the kinetic energy part would distribute the wave function amplitudes among different states in a completely **isotropic manner**.
Therefore, this description is analogous to a **directed random walk on a fully connected graph** where different nodes refer to the different states in superposition.

The starting recipe to this approach is the trotterization of the Schrödinger's wave equation, which is analogous to the diffusion equation with absorption (due to the potential energy component).

Since $i\frac{d}{dt}\psi(t+\Delta t) = H\psi(t+\Delta t)$,

$$\psi(\mathbf{t}+\mathbf{\Delta t}) = \mathbf{exp}(-\mathbf{iH\Delta t})\psi(\mathbf{t}) = \mathbf{U_H}\psi(\mathbf{t})$$

without loss of generality, let $\mathbf{H} = \mathbf{A} + \mathbf{B}$

$$\text{therefore, } exp(-i(A+B)\Delta t) \approx exp(-iA\Delta t)exp(-iB\Delta t) \textbf{ for small } \Delta t$$

Let $D = exp(-iA\Delta t)$ and $R = exp(-iB\Delta t)$.

Usually such approximations up to higher order terms are made for small time steps to minimize errors due to discretization.
**But Grover decided to use this Trotter approximation for the largest possible time step such that the condition of unitary evolution (i.e. $D^2 = I$ and $R^2 = I$) holds true.**

Intuitively, this means that the unitary evolution (norm preserving) for the largest time step should rotate some specific initial state on (or inside) the Bloch sphere as far as possible. **This farthest state is of course the state diametrically opposite to that initial state.**

**Therefore, the largest time step that allows $D$ and $R$ to be unitary is such that they become reflection operators.** This reflection operator condition on $D$ and $R$ **implies that A and B are projection operators** because, in general,

$$U_r = \pm(I - 2P) = \pm exp(\pm i\pi P).$$

For any reflection operator: $U_r^2 = I$, and some projection operator: $P^2 = P$.

**The composed transformation ($\mathbf{U_G} = \mathbf{DR}$) forms the state-transition transformation matrix for the finite step $\Delta t$.** Also clearly, $\mathbf{\Delta t} = \pi$.

The kinetic energy part ($A$) of the Hamiltonian ($H$) that diffuses the wave function amplitudes equally from one state to all other states is realised by the projection operator ($A = |s><s|$ where $|\mathbf{s}>=|\mathbf{0}>^{\otimes \mathbf{n}}$, and $n$ **is the number of qubits**) corresponding to the uniform superposition state.

Therefore, $\mathbf{D = 2|s><s| - I}$.

**The transition probability to go from state $|i>$ to state $|j>$ is** therefore,

$$< i|A|j >=< i|s >< s|j >= \mathbf{\frac{1}{N}} \text{ (where } N = 2^n)$$

**Hence, this is a completely unbiased and isotropic choice of wave function amplitude diffusion.**

The potential energy part ($B$) of the Hamiltonian ($H$) that attracts the system towards the target solution is the projection operator ($B = |t >< t|$) corresponding to the target state.

Now upon using our choice of isotropic diffusion operator ($D$) on the system, **the maximum transfer of wave function amplitude to the target state ($|t>$) takes place if a phase difference of $e^{i\pi} = -1$ (with respect to other states) is selectively applied the to $|t>$ before applying $D$.**

Therefore, $\mathbf{R = I - 2|t><t|}$.

In a continuous ideal description of unitary evolution, we can precisely evolve $|s>$ to $|t>$ under the action of $U_H(t)$ for some finite time ($t = t_H$).
Grover, on the other hand, intuitively decided to use the Trotter approximation for the largest time step possible which resulted in $D$ and $R$ to be reflection operators and $\Delta t = \pi$. The problem now reduces to finding how many iterations ($Q$) of $U_G = DR$ must be applied to $|s>$ so that

$$\mathbf{(U_G)^Q|s> \approx |t> \text{ or } | < t|(U_G)^Q|s> |^2 \approx 1}$$

It can be shown that $\mathbf{Q \approx \frac{\pi}{4}\sqrt{N}}$

Like in any Quantum Mechanical problem, the kinetic (a Laplacian) and potential (position dependent) energy terms do not commute, i.e. $\mathbf{[A, B] \neq 0}$
**Therefore for the case of large $\Delta t$, $\mathbf{U_H \neq DR}$.**

The effective Hamiltonian ($H_G$) corresponding to the Grover evolution ($U_G$), can thus be found out since,

$$\mathbf{U_G = DR = exp(-i\tau H_G)}$$

It can be shown that $\mathbf{H_G = i[|t><t|, |s><s|] = i[B, A]}$ and corresponding $\tau = \mathbf{\frac{2N}{\sqrt{N-1}} \sin^{-1}(\frac{1}{\sqrt{N}})}$

**Grover's adventurous intuition to choose the unitary evolution using the largest possible time step produced a surprising feature.**

**$|s>$ can taken to $|t>$ through unitary evolution paths of different Hamiltonian operators**, for example $H$ **for time** $t_H$ or $H_G$ **for time** $t_G = \tau\mathbf{Q}$ or any through other path on the **Bloch sphere (spanned by $|t>$ and $|t_\perp >= |s> - |t>$)** using any other suitable Hamiltonian.

It turns out that the choice of $H_G$ for finding the target state ($|t>$) from uniform superposition state ($|s>$) is the optimal solution which can be proved using variational analysis.

**Thus Grover's algorithm is the optimal solution to the search problem.**

Rarely, does it happen that crude intuition leads to the development of an algorithm that is not just efficient but optimal.
**This is the genius of Grover's algorithm!**

Next the code here discusses how this Search Algorithm can be run on a Quantum Database!