Quantum Machine Learning Seminars

Week 4: Quantum Algorithms

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Outline

1. Grover's Search Algorithm
2. Quantum Fourier transform
3. QML toolkit

The SAT Problem

- Boolean Satisfiability is a decision problem (yes, no) that checks if there exists some logical formula $F(x_1, \cdots, x_n) = 1$ for different n-variables $(x_1, \cdots x_n) \in \{0,1\}^n$. Classically this is an $\mathcal{NP}$ problem with brute force $\mathcal{O}(2^n)$.
- Example of $F(x_1, \cdots, x_n)$ is CNF-SAT $F = C_1 \wedge \cdots \wedge C_m$ where $C_i = \ell_1 \vee \cdots \vee \ell_k$ and $\ell_i \in \{x_i, \neg x_i\}$.
- For large "unstructured" database with N items, each database check is called query. And query complexity is $\Theta(N)$. For a classical SAT problem $\Theta(2^n)$ assuming the existence of a "unique" solution.

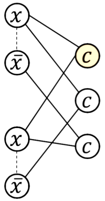
$$(x_1 \vee x_2) \wedge (x_1 \vee \neg x_2) \wedge (\neg x_1 \vee x_2)$$

Literals: $x_1, \neg x_1, x_2, \neg x_2$

Clauses: c_1, c_2, c_3

$$\Updownarrow$$

Bipartite graph



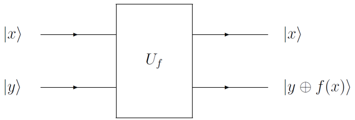
https://snap.stanford.edu/g2sat/

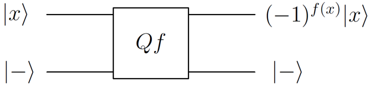
Grover's Oracle

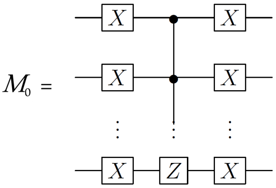
- If $\{x_i\}^n$ is basic encoded $|\psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle$ (how?) and is inspected to find $|x_0\rangle$, then the inner product and the constant probability of finding the state tell $\Theta(N) = \Theta(\sqrt{2^n})$.
- The classical search acts as $f : B_n \to B$ such that

$$f(x) = \begin{cases} 0 \ , & x \neq x_0, \\ 1 \ , & x = x_0. \end{cases} .$$

- In quantum regimes $f(x)$ becomes $U_f : |x\rangle|y\rangle \to |x\rangle|y \oplus f(x)\rangle$, where $|x\rangle$ is a control n-qubits and $|y\rangle$ is a target 1-qubit.





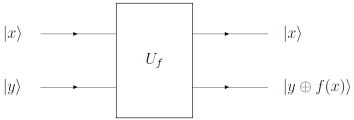


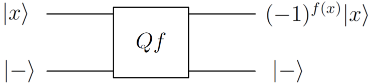
Grover's Iteration Operator

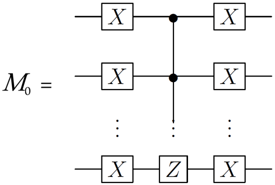
- Define $U_f : |x\rangle \to (-1)^{f(x)}|x\rangle$.
- To find $|x_0\rangle$ we use $M_{x_0} = \mathbb{1}_n - 2|x_0\rangle\langle x_0|$ such that

$$M_{x_0}|x\rangle = \begin{cases} +|x\rangle \ , \ x \neq x_0 \\ -|x\rangle \ , \ x = x_0 \end{cases} \equiv U_f|x\rangle.$$

- Show that $Qf(|x\rangle \otimes |-\rangle) = (-1)^{f(x)}|x\rangle|-\rangle$.
- So the entire process is handled using $G = H^{\otimes n} M_0 H^{\otimes n} U_f$.
- Repeated action of G would give either projected or reflected state until it finds $|x_0\rangle$.



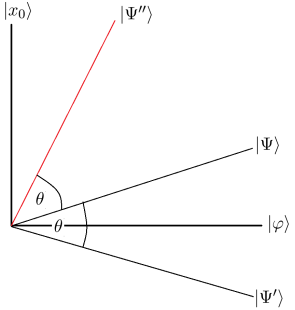




Grover's Search Algorithm

Angle encoding

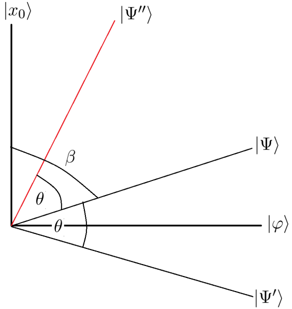
- After preparing $|\Psi\rangle = H^{\otimes n}|0\rangle$, define $|\Psi\rangle = \sin(\theta/2)|x_0\rangle + \cos(\theta/2)|\varphi\rangle$, where $\sin(\theta/2) = 1/\sqrt{2^n}$ and $|\varphi\rangle = \frac{1}{\sqrt{2^n-1}} \sum_{x \neq x_0} |x\rangle$.
- $U_f|\Psi\rangle$ gives $-|x_0\rangle$, i.e., reflects $|\Psi\rangle$ across $|\varphi\rangle$ to $|\Psi'\rangle$.
- Rather than using M_0, we use $-M_\Psi$, i.e., reflects the new state $|\Psi'\rangle$ across $|\Psi\rangle$ to get $|\Psi''\rangle$.
- Repeat and notice $|\Psi\rangle \to |x_0\rangle$ until they coincide.
- $G^k|\Psi\rangle \to |\Psi_f\rangle = \sin[(k+1)\frac{\theta}{2}]|x_0\rangle + \cos[(k+1)\frac{\theta}{2}]|\varphi\rangle$, with $\mathbb{P}_k(x_0) = \sin^2[(k+1)\frac{\theta}{2}]$, i.e., when $\boxed{k = \frac{\pi}{2}\sqrt{2^n} - 1 \Rightarrow |\Psi\rangle = |x_0\rangle}$, matching $\mathcal{O}(\sqrt{2^n})$.



Grover's Search Algorithm

2-Qubits $\Theta(\sqrt{2^2})$

- Define $\cos(\beta) = \langle x_0|\Psi\rangle = \frac{1}{\sqrt{2^n}}$.
- $k = \dfrac{\beta}{\theta/2}$.
- for 2-qubits, i.e., 4-items database, $\cos\beta = \frac{1}{\sqrt{2^2}} = \frac{1}{2} \Rightarrow \beta = \pi/3$ and $\theta/2 = \pi/3$.
- $\therefore k = 1$, i.e., $\Theta(\sqrt{N}) = 1$ You need only one query to make $|\Psi\rangle \to |x_0\rangle$.



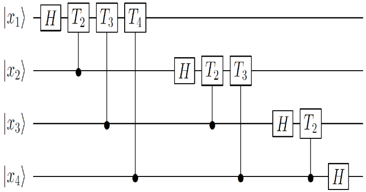
Amplitude Amplification

- It's a generalization of the Grover's algorithm where we search for M items rather than only 1, hence $\mathcal{O}(\sqrt{N/M})$.
- Given $f : X \to \{0,1\}$ with target set $T = \{x \in X : \ f(x) = 1\}$, define the good subspace $\mathtt{H}_g := \mathrm{span}\{|x\rangle \in \mathtt{H} : \ x \in T\}$, and the bad subspace $\mathtt{H}_b := \mathtt{H}_g^{\perp}$.
- Decompose $|\psi\rangle \in \mathtt{H}$ into good/bad components as $|\psi\rangle = \sin\theta\,|\varphi_g\rangle + \cos\theta\,|\varphi_b\rangle, \qquad \theta \in [0, \pi/2]$, with $|\varphi_g\rangle \in H_g$ and $|\varphi_b\rangle \in H_b$.
- Define $U_\psi := \mathbb{1} - 2|\psi\rangle\langle\psi|, \qquad U_g := \mathbb{1} - 2\sum_{x\in T} |x\rangle\langle x|$, where U_ψ flips the phase of $|\psi\rangle$ and U_g flips the phase of all states in $\mathtt{H}_g$; then set the Grover-like iterate $U := -U_\psi U_g$,
- $U|\psi_g\rangle = \cos(\theta)\,|\psi_g\rangle - \sin(\theta)\,|\psi_b\rangle, \qquad U|\psi_b\rangle = \cos(\theta)\,|\psi_b\rangle + \sin(\theta)\,|\psi_g\rangle$.
  $U^k|\psi\rangle = \sin\big((k+1)\theta/2\big)\,|\psi_g\rangle + \cos\big((k+1)\theta/2\big)\,|\psi_b\rangle$.

Quantum Fourier transform

Amplitude Encoding

- The discrete Fourier transform (DFT) is a map $\mathcal{F} : \mathbb{C}^N \to \mathbb{C}^N$ defined by:
  $\mathcal{F} : (\alpha_0, \ldots, \alpha_{N-1}) \longmapsto (\beta_0, \ldots, \beta_{N-1})$,
  $\beta_y := \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \alpha_x \, e^{i\left(\frac{2\pi}{N} xy\right)}$.
- Adopting amplitude encoding with $N = 2^n$, QFT is a unitary U_F acting on an n-qubit register as:
  $U_F \left[\sum_{x=0}^{2^n-1} \alpha_x |x\rangle\right] = \sum_{y=0}^{2^n-1} \beta_y |y\rangle$.
- Since α_x isn't physical, so is β_y. Thus QFT needs to be part of a larger quantum algorithm like Quantum phase estimation.

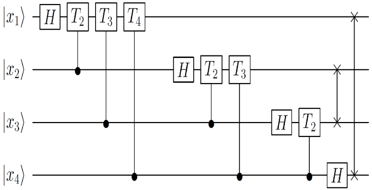


Quantum Fourier transform

Amplitude Encoding

- $T_k := P_{\frac{2\pi}{2^k}}$ for $k = 1, 2, 3, 4.$:
- $T_4T_3T_2H|x_1\rangle = T_4T_3T_2\frac{|0\rangle+(-1)^{x_1}|1\rangle}{\sqrt{2}} =$

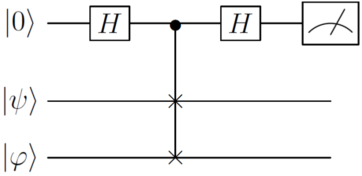
  $T_4T_3\frac{|0\rangle+e^{i\pi x_1+i\frac{\pi}{2}x_2}|1\rangle}{\sqrt{2}} = \frac{|0\rangle+e^{i2\pi\sum_{j=1}^{4}\frac{x_j}{2^j}}|1\rangle}{\sqrt{2}} = \frac{|0\rangle+e^{i\frac{2\pi x}{2^4}}|1\rangle}{\sqrt{2}}.$
- $T_3T_2H|x_2\rangle = \frac{|0\rangle+e^{i\frac{2\pi x}{2^3}}|1\rangle}{\sqrt{2}}.$
- $T_2H|x_3\rangle = \frac{|0\rangle+e^{i\frac{2\pi x}{2^2}}|1\rangle}{\sqrt{2}}.$
- $H|x_4\rangle = \frac{|0\rangle+e^{i\frac{2\pi x}{2}}|1\rangle}{\sqrt{2}}.$



QML toolkit

SWAP test

- For $|\psi\rangle$ and $|\varphi\rangle$ "unknown" pure state.
- $|\Psi\rangle = (H\otimes I\otimes I)F(H\otimes I\otimes I)|0,\ \psi,\ \varphi\rangle =$
$(H\otimes I\otimes I)F|+,\ \psi,\ \varphi\rangle$
$= (H\otimes I\otimes I)\frac{1}{\sqrt{2}}\Big(|0,\ \psi,\ \varphi\rangle + |1,\ \varphi,\ \psi\rangle\Big) =$
$\frac{1}{2}|0\rangle\big(|\psi\ \varphi\rangle + |\varphi\ \psi\rangle\big) + \frac{1}{2}|1\rangle\big(|\psi\ \varphi\rangle - |\varphi\ \psi\rangle\big)$.
- The probability to measure 0 on the first qubit is:
$\mathbb{P}(0) = \langle\Psi|\big((|0\rangle\langle 0|\otimes I\otimes I)\big)|\Psi\rangle =$
$\frac{1}{4}\big(\langle\psi\varphi| + \langle\varphi\psi|\big)\big(|\psi\varphi\rangle + |\varphi\psi\rangle\big)$
$= \frac{1}{2} + \frac{1}{4}\Big(\langle\psi|\varphi\rangle\langle\varphi|\psi\rangle + \langle\varphi|\psi\rangle\langle\psi|\varphi\rangle\Big) = \frac{1}{2} + \frac{1}{2}|\langle\psi|\varphi\rangle|^2$.
- Thus it's useful for measuring angles between these unknown states.



QML toolkit

Qdist routine

- Use amplitude encoding for real vectors $\mathbf{x} \in \mathbb{R}^d$, encode it into a $\log d$-qubit as $|\mathbf{x}\rangle = \frac{1}{|\mathbf{x}|}\sum_{j=1}^{d} x_j |j\rangle$.
- For two real vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, the overlap of their amplitude-encoded states gives: $\langle \mathbf{x}|\mathbf{y}\rangle = \cos(\mathbf{x}, \mathbf{y}) = \dfrac{\mathbf{x}\cdot\mathbf{y}}{|\mathbf{x}||\mathbf{y}|}$.
- Prepare an entangled state with the data register, $|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|0\rangle \otimes |\mathbf{x}\rangle + |1\rangle \otimes |\mathbf{y}\rangle\Big) \in \mathbb{C}^2 \otimes (\mathbb{C}^2)^{\otimes n}$, then another state $|\varphi\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle - |1\rangle\big) \in \mathbb{C}^2$.
- Check the overlap with the ancilla $|\varphi\rangle$ to get $\Phi = \frac{1}{\sqrt{2}}\big(\langle\varphi|0\rangle|\mathbf{x}\rangle + \langle\varphi|1\rangle|\mathbf{y}\rangle\big) = \frac{1}{\sqrt{2}}\big(|\mathbf{x}\rangle - |\mathbf{y}\rangle\big)$.
- SWAP to estimate $|\Phi|^2$, and $|\Phi|^2 = 1 - \frac{\mathbf{x}\cdot\mathbf{y}}{|\mathbf{x}||\mathbf{y}|}$. Hence $\mathbf{x}\cdot\mathbf{y} = (1 - |\Phi|^2)|\mathbf{x}||\mathbf{y}|$, and the squared distance is $|\mathbf{x}-\mathbf{y}|^2 = |\mathbf{x}|^2 + |\mathbf{y}|^2 - 2\mathbf{x}\cdot\mathbf{y}$.

Thank You!