Global Optimum Search in Quantum Deep Learning

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Project of CS 880: Quantum Computing

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Overview

Gradient Descent

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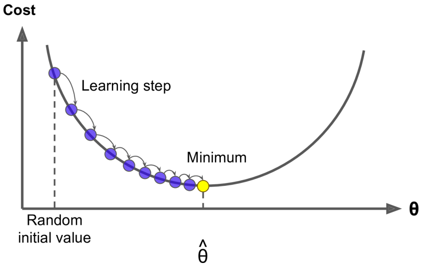
$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{L}(\theta)$$

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{j=1}^{N} \ell(\theta, x_j)$$

$$\theta_{k+1} = \theta_k - \eta \frac{\partial \mathcal{L}_\theta}{\partial \theta}\bigg|_{\theta=\theta_k}$$



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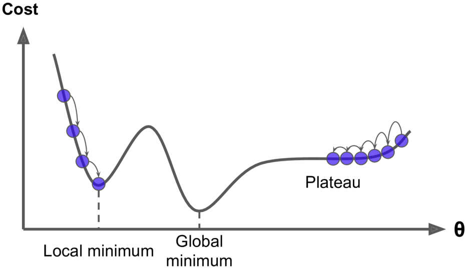

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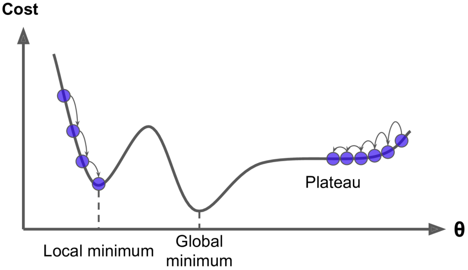

- The upper bound or expected number of iterations to reach convergence is difficult to determine.

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- Theoretical analyses to show that the expected cost for both approaches are $O(\sqrt{|\Theta|}N)$.
- Novel objective function maximizing the number of "cut-off indicators $\mathbb{E}_{\theta j}$" to fit the property of quantum computing in optimizing machine learning models
- Potential for PSTC to reduce the cost further to $O(\sqrt{|\Theta|} \cdot sublinear(N))$ in future work

Overview of Average Approach

$$|\theta\rangle|j\rangle|\mathbf{0}\rangle \xmapsto{\text{Quantum parallelism with cost } O(N)} |\theta\rangle|j\rangle|\sum_{j=1}^{N}\ell(\theta, x_j)\rangle$$

$$\theta^*_{avg} = \operatorname*{argmin}_{\theta\in\Theta} \mathcal{L}_\theta^{avg} = \operatorname*{argmin}_{\theta\in\Theta} \frac{1}{N}\sum_{j=1}^{N}\ell(\theta, x_j)$$

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- Treat the machine learning model as a quantum blackbox
- Utilize Durr & Hoyer (DH) algorithm to find the global minimum
- Expected number of steps: $O(N\sqrt{|\Theta|})$

Overview of Partial Swap Test Cut-off (PSTC) Approach

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- Employ a "partial" swap test and amplitude amplification to boost the probability of finding a good θ
- Still $O(N\sqrt{|\Theta|})$, but only at checking process
- Enable future improvement to maybe $O(sublinear(N) \cdot \sqrt{|\Theta|})$

Overview

Approach 1: Average Approach

1. Consider the function $f(i) = f(\theta_i) := \sum_j \ell(\theta_i, x_j)$
2. Use the DH algorithm [2] to find the minimum of the set $\{f(i)\}_i$ with a slight modification: When the DH algorithm queries $f(i)$ for some i (i.e. when the algorithm makes a query on $|i\rangle|0^t\rangle$ and needs $|i\rangle|f(i)\rangle$ as output), do the following subroutine:
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   - Return $U(|i\rangle|0^t\rangle)$ to the DH algorithm.

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- So, the cost is $O(\sqrt{|\Theta|}N)$.
- Also, we know that the DH algorithm succeeds with probability 0.5 and so by running it many times, we get the parameter minimizing the loss with arbitrarily good accuracy at the cost $O(\sqrt{|\Theta|}N)$.

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- Want some function f: $\sum_{j=1}^{N} |\theta\rangle|j\rangle|\mathbf{0}\rangle \xmapsto{\text{Cost } O(1)} \sum_{j=1}^{N} |\theta\rangle|j\rangle|f(\theta, x_j)\rangle$

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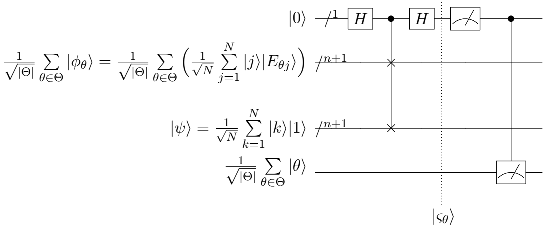

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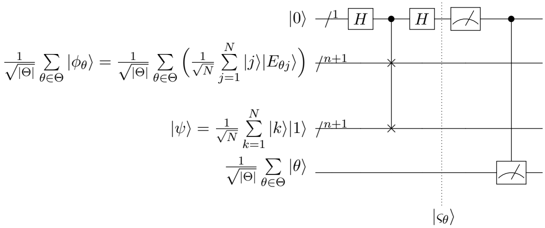

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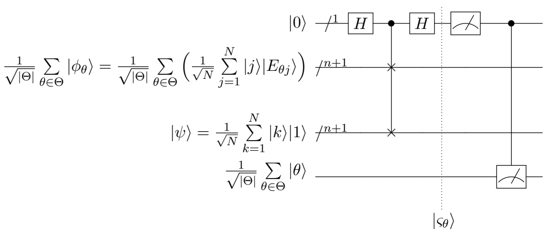

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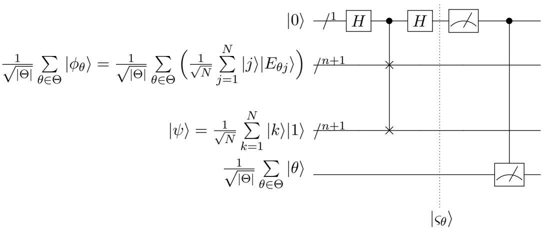

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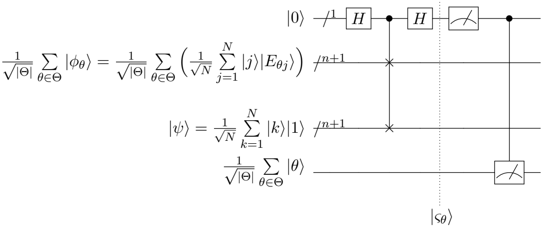

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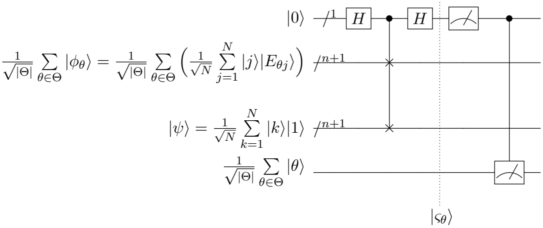

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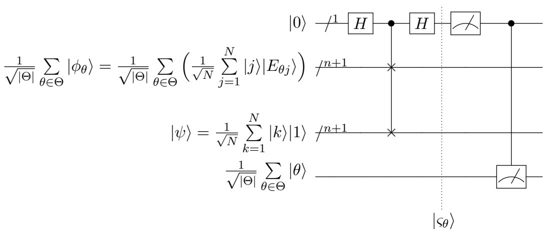

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- Want larger $\mathcal{L}_\theta^{\text{PSTC}}$
- **The better θ we want, the higher chance we can observe θ!**

$\mathcal{A}_{\text{Boost}}$: Amplitude Amplification

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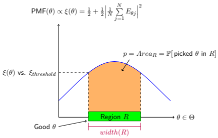
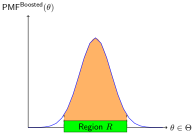
Table: Amplitude amplification for the PMF$(\theta) \propto \xi(\theta)$





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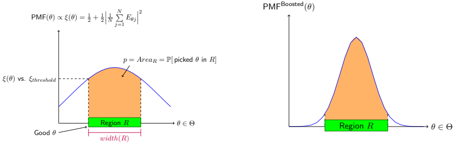

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- In the manner $\sim$ Grover's Search [1]

$$\#(Q_{\text{1-query}}) = O(\tfrac{1}{p}) \quad \xmapsto{\;improved\;} \quad \#(Q_{\text{1-query}}) = O(\tfrac{1}{\sqrt{p}})$$

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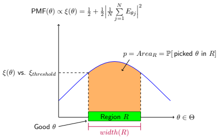

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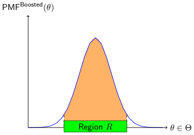

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- Checking process: To determine whether $\theta \in R$

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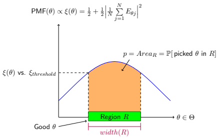

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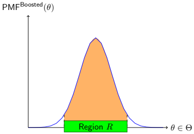

After $\mathcal{A}_{\text{Boost}}$

$$p = Area_R = \mathbb{P}[\,\text{picked } \theta \text{ in } R]$$

- In the manner $\sim$ Grover's Search [1]

$$\#(Q_{\text{1-query}}) = O(\tfrac{1}{p}) \text{ via classic algorithm} \xmapsto{improved} \#(Q_{\text{1-query}}) = O(\tfrac{1}{\sqrt{p}}) \text{ via } \mathcal{A}_{\text{Boost}}$$

- Checking process: To determine whether $\theta \in R \leftarrow$ Cost $O(N)$

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- $\because$ Region R in later iteration is narrower than the previous iterations

i.e. $Cost_{\text{Final iteration}}+...+Cost_{\text{1st iteration}} = O(\sqrt{|\Theta|}+\frac{\sqrt{|\Theta|}}{2}+\frac{\sqrt{|\Theta|}}{4}+...) = O(\sqrt{|\Theta|})$

Overview

Equivalency Discussion

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- I.e., are there constants C, c such that on any sample set and any choice of ℓ,
$$c\theta^*_{PSTC} \leq \theta^*_{avg} \leq C\theta^*_{PSTC}.$$

Equivalency Discussion

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- So, $C+1 \leq C$ gives a contradiction.

Overview

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- Future work: to lower the cost of PSTC to $O(\sqrt{|\Theta|} \cdot sublinear\ N)$ by enhancing the checking process

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- In view of this, we can generalize the cut-off indicator $E_{\theta j}$ to ${E^{A}}_{\theta j}$:

$$\mathcal{L}_{\theta}^{A,\mathsf{PSTC}} \triangleq \frac{1}{N} \sum_{j=1}^{N} {E^{A}}_{\theta j}, \text{ where } {E^{A}}_{\theta j} = \mathbb{1}[\,\ell(\theta, x_j) \leq \tilde{\ell} \text{ and } \theta \in A]$$

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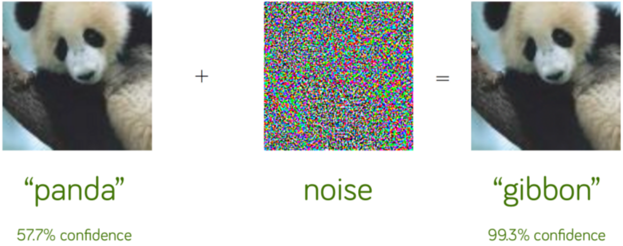

$$x + \delta^{adv} = x^{adv}$$

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- Apply PSTC by searching for "good" $\delta \in X$ and we will be able to obtain an adversarial example in the cost of $O(\sqrt{|X|})$.

Thank you!

Overview

Notations Table: Basics

Notation	Space	Meaning
θ	Θ	Parameter of model $h_\theta(\cdot)$
$h_\theta(\cdot)$	$X \to Y$	Model with parameter θ
x	X	An input
y	Y	A label
S	$S \subseteq X$	$\{x_1, ..., x_N\}$
N	$\mathbb{Z}^+$	$\#$(samples in S)
n	$\mathbb{Z}^+$	$N = 2^n$
m	$\mathbb{Z}^+$	$\lvert\Theta\rvert = 2^m$
$\ell(\cdot,\cdot)$, or $loss(\cdot,\cdot)$	$\Theta \times X \to \mathbb{R}^+$	Loss function
	(or $Y \times Y \to \mathbb{R}^+$)	(depending on context)
ℓ_{ij}, or $\ell_{\theta_i j}$, or $\ell_{\theta j}$	$\mathbb{R}^+$	$\ell_{\theta_i j} = \ell(\theta_i, x_j) = \ell(h_{\theta_i}(x_j), y_j)$
$\mathcal{L}_\theta^{avg}$ or $\mathcal{L}^{avg}(\theta)$	$\mathbb{R}^+$	Average loss $\frac{1}{N}\sum_{j=1}^{N} \ell_{\theta j}$; The smaller the better
$\mathcal{L}_\theta^{\text{PSTC}}$ or $\mathcal{L}^{\text{PSTC}}(\theta)$	$\mathbb{R}^+$	Cut-off loss $\frac{1}{N}\sum_{j=1}^{N} \mathbb{1}[\ell_{\theta j} \le \tilde{\ell}]$; The larger the better
$\tilde{\ell}$, or $\ell_{threshold}$	$\mathbb{R}^+$	Threshold value for the cut-off approach
$E_{\theta j}$	$\{0,1\}$	Cut-off indicator: Value $\mathbb{1}[\ell_{\theta j} \le \tilde{\ell}]$ to be stored in 1 qubit
$\lvert\phi\rangle, \lvert\psi\rangle$	$\mathbb{C}^{n+1}$	Pure states used in PSTC

Notations Table: PSTC

$Q_{\text{1-query}}$	Q-Circuits	The Q-circuit for partial swap test
$\lvert\varsigma_\theta\rangle$	$\mathbb{C}^{2n+3}$	The pure state after the 2nd Hadamard gate in $Q_{\text{1-query}}$ given θ
$\lvert\varsigma_\theta^{(0)}\rangle, \lvert\varsigma_\theta^{(1)}\rangle$	$\mathbb{C}^{2n+2}$	The $\lvert 0\rangle$ and $\lvert 1\rangle$ parts of $\lvert\varsigma_\theta\rangle$
PMF$(\cdot)$	$\Theta \to [0,1]$	Probability mass function (PMF) of θ
$\mathcal{A}_{\text{1-query}}$, $\mathcal{A}_\xi$, $\mathcal{A}_{\text{Boost}}$, $\mathcal{A}_{\text{PSTC}}$	Algorithms	Names of some cut-off approach algorithms
$\theta_{\text{1-query}}$, θ_{Boost}, θ_{Best}	Θ	θ being used in the respective algorithms
$flag(\cdot)$	$\Theta \to \{0,1\}$	Flag to indicate whether θ is good or bad
O_{flag}	$\mathbb{C}^{m\times m}$	Gate of oracles on $flag(\theta)$
$\mathcal{R}$	$\mathbb{C}^{m\times m}$	Gate of "keeping zero, flipping else"
R	$R \subseteq \Theta$	Region R that "good" θs concentrate
$ref(\lvert B\rangle)$	$\mathbb{C}^{m\times m}$	Reflection on the "Bad" vector in $\mathcal{A}_{\text{Boost}}$
$ref(\lvert U\rangle)$	$\mathbb{C}^{m\times m}$	Reflection on the "Uniform" vector in $\mathcal{A}_{\text{Boost}}$
p	$[0,1] \in \mathbb{R}$	$\mathbb{P}[$picked θ in $R]$
$\xi(\cdot)$	$\Theta \to \mathbb{R}^+$	A function that proportional to pdf of θ : $P[$observe $\theta\rvert$1st qubit $=0]$
$\tilde{\xi}$, or $\xi_{threshold}$	$\mathbb{R}^+$	Threshold value of ξ for region R
$\lvert\mathbf{0}\rangle$	$\mathbb{C}^{\text{not care}}$	High dimensional $\lvert 0\rangle$ with dimension not mentioned
x^{adv}	X	Adversarial example
δ^{adv}	X	Perturbation
$\lvert\chi^{\text{Type I}}\rangle$, $\lvert\chi^{\text{Type II}}\rangle$	$\mathbb{C}^{\text{depends}}$	Pure states of x referring to Type I and Type II uniformity.

References

[1] R. de Wolf. Quantum computing: Lecture notes, 2019. URL https://arxiv.org/abs/1907.09415.

[2] C. Durr and P. Hoyer. A Quantum Algorithm for finding the Minimum. 1999. URL https://arxiv.org/abs/quant-ph/9607014.