Provable Quantum Speed-ups for Optimization and Machine Learning

Xiaodi Wu

Based on (1) arXiv:1809.01731v1 (QIP 2019);
(2) arXiv:1710.02581v2 (QIP 2019);
Outline

Motivation

Convex Optimization

Semidefinite programs

Classification

Lower bounds

Future research
Optimization and Machine Learning – two sides of the same coin!
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Quantum Speed-up for Optimization and Machine Learning

one of important quantum applications.
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Heuristic: variational, annealer, QAOA, ....
Interplay: Quantum, Optimization & Machine Learning

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- **Heuristic**: variational, annealer, QAOA, ....
- **Provable**: (1) thorough understanding of heuristics; (2) valuable guideline when empirical results are scarce.
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- one of important quantum applications.
- **Heuristic**: variational, annealer, QAOA, ....
- **Provable**: (1) thorough understanding of heuristics; (2) valuable guideline when empirical results are scarce.
- This talk focuses on *quantization* of classical algorithms.
Quantization of Classical Algorithms

A typical classical iterative algorithm:

- Assume a feasible set $P$. Want to optimize $f(x)$ s.t. $x \in P$.
- A generic iterative algorithm with $T$ iterations:
  - $x_1 \rightarrow x_2 \rightarrow \cdots \rightarrow x_T$. Cost for each step: (1) store $x_i$; (2) determine $x_i$ based on $x_{i-1}, \cdots, x_1, P, f(x)$.

How quantum potentially speeds up this procedure?

- Reduce the cost for each step. Make it quantum and/or store $x_i$ quantumly. However, this could complicate the determination of next $x_i$.
- Not clear how to reduce the number of iterations $T$. 
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Cases where we can make it work

- **Convex Optimization**: a quantum algorithm using $\tilde{O}(n)$ queries to the *evaluation* and the *membership* oracles, whereas the best known classical algorithms makes $O(n^2)$ such queries.
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- **Quantum SDP solvers**: a quantum algorithm solves $n$-dimensional semidefinite programs with $m$ constraints, sparsity $s$ and error $\epsilon$ in time $\tilde{O}((\sqrt{m} + \sqrt{n})s^2(Rr/\epsilon)^8)$, where $R, r$ are bounds on the primal/dual solutions.
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- **Classification**: a sublinear quantum algorithm for training linear and kernel-based classifiers that runs in $O(\sqrt{n} + \sqrt{d})$ given $n$ data points in $\mathbb{R}^d$, whereas the state-of-the-art (and optimal) classical algorithm runs in $O(n + d)$. 
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Yes, we do have accompanying lower bounds.
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Convex optimization

Convex optimization is a central topic in computer science with applications in:

- **Machine learning**: training a model is equivalent to optimizing a loss function.
- **Algorithm design**: LP/SDP-relaxation, such as various graph algorithms (vertex cover, max cut, ...)
- ......

Classically, it is a major class of optimization problems that has polynomial time algorithms.
Convex optimization

In general, convex optimization has the following form:

\[
\min f(x) \quad \text{s.t. } x \in \mathcal{C},
\]

where \( \mathcal{C} \subseteq \mathbb{R}^n \) is promised to be a convex body and \( f : \mathbb{R}^n \to \mathbb{R} \) is promised to be a convex function.
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It is common to be provided with two oracles:

- *membership oracle*: input an $x \in \mathbb{R}^n$, tell whether $x \in \mathcal{C}$;
- *evaluation oracle*: input an $x \in \mathcal{C}$, output $f(x)$. 
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Given a parameter $\epsilon > 0$ for accuracy, the goal is to output an $\tilde{x} \in \mathcal{C}$ such that

$$f(\tilde{x}) \leq \min_{x \in \mathcal{C}} f(x) + \epsilon.$$
Convex optimization

Classically, it is well-known that such an $\tilde{x}$ can be found in polynomial time using the ellipsoid method, cutting plane methods or interior point methods.
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Currently, the state-of-the-art result by Lee, Sidford, and Vempala uses \( \tilde{O}(n^2) \) queries and additional \( \tilde{O}(n^3) \) time.
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Currently, the state-of-the-art result by Lee, Sidford, and Vempala uses $\tilde{O}(n^2)$ queries and additional $\tilde{O}(n^3)$ time.

Quantumly, we are promised to have unitaries $O_C$ and $O_f$ s.t.
- for any $x \in \mathbb{R}^n$, $O_C |x\rangle|0\rangle = |x\rangle|I_C(x)\rangle$, where $I_C(x) = 1$ if $x \in C$ and $I_C(x) = 0$ if $x \notin C$;
- for any $x \in C$, $O_f |x\rangle|0\rangle = |x\rangle|f(x)\rangle$. 
Main result. Convex optimization takes

- $\tilde{O}(n)$ and $\Omega(\sqrt{n})$ quantum queries to $O_C$;
- $\tilde{O}(n)$ and $\tilde{\Omega}(\sqrt{n})$ quantum queries to $O_f$.

Furthermore, the quantum algorithm also uses $\tilde{O}(n^3)$ additional time.
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As a result, we obtain:

- The first nontrivial quantum upper bound on general convex optimization.
- Impossibility of generic exponential quantum speedup of convex optimization! The speedup is at most polynomial.
Convex optimization: quantum upper bound

Lee-Sidford-Vempala gives classical oracle reductions:

\[ \tilde{O}(n) \]

Both papers use the same cutting plane based reduction from OPT to SEP. We show an improved upper bound by reducing the query complexity of the reduction from SEP to MEM.
Convex optimization: quantum upper bound

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We give corresponding quantum oracle reductions:

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Construction of SEP from MEM

- A $O(n)$ classical reduction w/ sub-gradient computation.
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Jordan’s algorithm for gradients!

- Prepare the state $e^{if(x)}|x\rangle$ with $\tilde{O}(1)$ queries.
- Since $f(x) \approx \sum_{k=1}^{n} \frac{\partial f}{\partial x_k} x_k,$

$$\sum_{x} e^{if(x)}|x\rangle \approx \sum_{x} \bigotimes_{k=1}^{n} e^{i \frac{\partial f}{\partial x_k} x_k} |x_k\rangle.$$  

Apply QFT reveals $\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_n}.$
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*From gradients to sub-gradients*

- Compute the gradient of the *mollification* of the original function!
- Achieve so by carefully sampling from the neighborhood.
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Semidefinite programming (SDP)

Given \( m \) real numbers \( a_1, \ldots, a_m \in \mathbb{R} \), \( s \)-sparse \( n \times n \) Hermitian matrices \( A_1, \ldots, A_m, C \), the SDP is defined as

\[
\begin{align*}
\max \quad & \operatorname{tr}[CX] \\
\text{s.t.} \quad & \operatorname{tr}[A_i X] \leq a_i \quad \forall i \in [m]; \\
& X \succeq 0.
\end{align*}
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SDPs can be solved in polynomial time. Classical state-of-the-art algorithms include:

- **Cutting-plane method:** $\tilde{O}(m(m^2 + n^{2.374} + mns) \text{ poly log}(Rr/\epsilon))$.
- **Matrix multiplicative weight:** $\tilde{O}(mns(Rr/\epsilon^7))$. 

Quantum algorithms for SDPs

Brandão and Svore gave a quantum algorithm with complexity $\tilde{O}(\sqrt{mns^2} (Rr/\epsilon)^{32})$, a quadratic speed-up in $m, n$, (later improved to $\tilde{O}(\sqrt{mns^2} (Rr/\epsilon)^8)$, based on the Matrix Multiplicative Weight Update method.
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Input model
An oracle that takes input $j \in [m + 1]$, $k \in [n]$, $l \in [s]$, and performs the map

$$|j, k, l, 0\rangle \mapsto |j, k, l, (A_j)_{k,s_{jk}}(l)\rangle,$$

where $(A_j)_{k,s_{jk}}(l)$ is the $l^{th}$ nonzero element in the $k^{th}$ row of matrix $A_j$. 
Optimal quantum algorithms for SDPs

Can we close the gap between $\tilde{O}(\sqrt{mn})$ and $\Omega(\sqrt{m} + \sqrt{n})$?
Optimal quantum algorithms for SDPs

Can we close the gap between $\tilde{O}(\sqrt{mn})$ and $\Omega(\sqrt{m} + \sqrt{n})$? Yes!

**Theorem**
For any $\epsilon > 0$, there is a quantum algorithm that solves the SDP using at most

$$\tilde{O}((\sqrt{m} + \sqrt{n})s^2(Rr/\epsilon)^8)$$

quantum gates and queries to oracles.
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Optimal quantum algorithms for SDPs

The behavior of the algorithm:

- **The good**: optimal in $m, n$
- **The bad**: dependence on $R, r, \epsilon^{-1}$ is too high: $(Rr/\epsilon)^8$
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Applications:

▶ The good: Some machine learning, especially compressed sensing problems have $Rr/\epsilon = O(1)$ (Ex. quantum compressed sensing by Gross et al. 09).
▶ The bad: The SDP in the Goeman-Williams algorithm for MAX-CUT has $Rr/\epsilon = \Theta(n)$ (and many other algorithmic SDP applications).
Matrix multiplicative weight method (MMW)

Versatile Framework

- MMW: (matrix) boosting, online learning, ....
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- A good candidate to quantize:
  - The number of iterations $T$ is poly-log in terms of $n$ and $m$. 

$\rho(t) = \exp\left[\sum_{\tau=1}^{t-1} \tau \right]$, which is a Gibbs state that quantumly can generate efficiently! (e.g., PW09)
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- A good candidate to quantize:
  - The number of iterations $T$ is poly-log in terms of $n$ and $m$.
  - Each intermediate solution is
    \[
    \rho(t) = \frac{\exp \left[ \frac{\epsilon}{4} \sum_{\tau=1}^{t-1} M^{(\tau)} \right]}{\text{Tr} \left[ \exp \left[ \frac{\epsilon}{4} \sum_{\tau=1}^{t-1} M^{(\tau)} \right] \right]},
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Consider the following SDP feasibility problem:

\[ \text{tr}[A_i X] \leq a_i + \epsilon \quad \forall \; i \in [m]; \quad (1) \]

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Zero-sum Game View

- Player 1: a feasible $X \in S_\epsilon$.
- Player 2: any violation of any proposed $X$. 

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An *equilibrium* point of such can be found by MMW.
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Efficiency of Implementation

- Player 1 is due to quantum Gibbs sampling.
- Player 2 is due to a faster quantum OR lemma.
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A visualization of classification

Given $X_1, \ldots, X_n \in \mathbb{R}^d$ and a label vector $y \in \{-1, +1\}^n$, find a hyperplane $w \in \mathbb{R}^d$, s.t. $y_i \cdot X_i^T w \geq 0$, $\forall i \in [n]$.

(Kernel-based) $X_i \rightarrow \Phi(X_i)$ for some kernel function $\Phi(\cdot)$. 
A visualization of classification

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Input/Output Model & Result

Input/Output Model

- (input) Standard coherent access to each entry of $X_i$.
- (output) Classical efficient representation of $w$ (recover any $w_i$ with $\tilde{O}(1)$ overhead).
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Result & Comparison

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Similar results apply to kernel-based classification, minimum enclosing ball, and $\ell_2$-SVM.
This is an *equilibrium value* problem in disguise. Take $X_i \leftarrow (-1)^{y_i} X_i$, it reduces to $\max_w \min_i X_i^\top w \geq 0$. However, this is an example over $\ell_2$ unit balls. Fortunately, there exists a classical $\ell_2$ sampling approach with $O(n + d)$ cost for multiplicative weight updates. (Analysis relies on martingale concentration bounds.) Extend $\ell_2$ sampling to quantum is equivalent to state preparation of particular quantum states. Main contributions:

- $O(\sqrt{n} + \sqrt{d})$ quantum sampling of the desired state.
- Extension of the concentration analysis to quantum.

Feature of the quantum algorithm classical output, highly classical-quantum hybrid, state sampling.
High-level Technique

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- Extend $\ell_2$ sampling to quantum is equivalent to *state preparation* of particular quantum states.
- Main contributions:
High-level Technique

- This is an *equilibrium value* problem in disguise. Take $X_i \leftarrow (-1)^{y_i} X_i$, it reduces to $\max_w \min_i X_i^\top w \geq 0$.
- However, this is an example over $\ell_2$ unit balls.
- Fortunately, there exists a classical $\ell_2$ *sampling* approach with $O(n + d)$ cost for multiplicative weight updates. (*analysis relies on martingale concentration bounds.*)
- Extend $\ell_2$ sampling to quantum is equivalent to *state preparation* of particular quantum states.
- Main contributions:
  - $O(\sqrt{n} + \sqrt{d})$ quantum sampling of the desired state.
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Feature of the quantum algorithm
classical output, highly classical-quantum hybrid, state sampling
Outline

Motivation

Convex Optimization

Semidefinite programs

Classification

Lower bounds

Future research
The lower bound

- **Convex Optimization**: Convex optimization takes
  - $\tilde{O}(n)$ and $\Omega(\sqrt{n})$ quantum queries to $O_C$;
  - $\tilde{O}(n)$ and $\tilde{\Omega}(\sqrt{n})$ quantum queries to $O_f$.

- **Semidefinite Programs**:
  - Upper bound: $\tilde{O}((\sqrt{m} + \sqrt{n})s^2(Rr/\epsilon)^8)$.
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**High-level difficulty:**

- (1) continuous domain (vs Boolean oracle query);
- (2) classical lower bounds are not studied comprehensively;
- (3) how to go beyond $\Omega(\sqrt{n})$?
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Continue on this thread:

- More quantization of classical MCMC algorithms (hitting or mixing)?

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- Non-convex optimization: (1) ubiquitous in ML; (2) numerical evidence of quantum speed-up. *Anything provable?*
Technical Open Questions I:

- Can we close the gap for both membership and evaluation queries? Our upper bounds on both oracles use $\tilde{O}(n)$ queries, whereas the lower bounds are only $\tilde{\Omega}(\sqrt{n})$.

- Can we improve the time complexity of our quantum algorithm? The time complexity $\tilde{O}(n^3)$ of our current quantum algorithm matches that of the classical state-of-the-art algorithm.

- What is the quantum complexity of convex optimization with a first-order oracle (i.e., with direct access to the gradient of the objective function)?
Technical Open Questions II:

- Concrete applications where quantum algorithms (both for convex optimization and SDPs) can have provable speed-ups?

- The use of QRAM (or non-trivial quantum data structure) in the state preparation steps in both quantum algorithms for SDPs and classification? Advantage for amortized complexity?

- Quantum algorithms for equilibrium point problems over other domain (e.g., game theory, learning theory)? The efficiency will depend on specific sampling techniques.
Thank you!

Q & A