How Quantum Computing Can Help With (Continuous) Optimization

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1. Known Advantages of Quantum Computing

- It is known that quantum computing enables us to drastically speed up many computations.

- One example of such a problem is the problem of looking for a given element in an unsorted $n$-element array.

- With non-quantum computations:
  - to be sure that we have found this element,
  - we need to spend at least $n$ computational steps.

- Indeed, if we use fewer than $n$ steps:
  - this would mean that we only look at less than $n$ elements of the array, and thus,
  - we may miss the element that we are looking for.
2. Advantages of Quantum Computing (cont-d)

- Grover’s quantum-computing algorithm allows us to reduce the time to $c \cdot \sqrt{n}$.

- So, we reduce the non-quantum computation time $T$ to
  
  $$T_q \sim \sqrt{T}.$$
3. Need to Consider Optimization Problems

- In many applications, we also need to solve continuous optimization problems.
- We want to find an object or a strategy for which the given objective function attains its maximum.
- An object is usually characterized by its parameters \( x_1, \ldots, x_n \).
- For each \( x_i \), we usually know the bounds: \( x_{i\text{\lowercase{}}} \leq x_i \leq x_{i\text{\uppercase{}}} \).
- Let \( f(x_1, \ldots, x_n) \) denote the value of the objective function corresponding to the parameters \( x_1, \ldots, x_n \).
- In most practical situations, the objective function is several (at least two) times continuously differentiable.
4. General Optimization Problem

- Ideal case: find $x_1^{\text{opt}}, \ldots, x_n^{\text{opt}}$ for which $f(x_1, \ldots, x_n)$ attains its maximum on the box

$$B \overset{\text{def}}{=} [x_1, \bar{x}_1] \times \ldots \times [x_n, \bar{x}_n].$$

- In practice, we can only attain values approximately.

- So, in practice, we are looking for the values $x_1^d, \ldots, x_n^d$ which are maximal with given accuracy $\varepsilon > 0$:

$$f(x_1^d, \ldots, x_n^d) \geq \left( \max_{(x_1, \ldots, x_n) \in B} f(x_1, \ldots, x_n) \right) - \varepsilon.$$

- We show that for this problem, quantum computing reduced computation time $T$ to $T_q \sim \sqrt{T} \cdot \ln(T)$. 
5. We Consider Only Guaranteed Global Optimization Algorithms

- Of course, there are many semi-heuristic ways to solve the optimization problem.
- For example, we can start at some point $x = (x_1, \ldots, x_n)$ and use gradient techniques to reach a local maximum.
- However, these methods only lead to a local maximum.
- If we want to make sure that we reached the actual (global) maximum:
  - we cannot skip some subdomains of the box $B$,
  - we have to analyze all of them.
- How can we do it?
6. Non-Quantum Lower Bound

- Let us select some size $\delta > 0$ (to be determined later).
- Let us divide each interval $[\bar{x}_i, x_i]$ into $N_i \overset{\text{def}}{=} \frac{\bar{x}_i - x_i}{\delta}$ subintervals of width $\delta$.
- This divides the whole box $B$ into $N = N_1 \cdot \ldots \cdot N_n = \prod_{i=1}^{n} \frac{\bar{x}_i - x_i}{\delta} = \frac{V}{\delta^n}$ subboxes.
- Here, $V$ is the volume of the original box $B$:
  \[ V \overset{\text{def}}{=} (\bar{x}_1 - x_1) \cdot \ldots \cdot (\bar{x}_n - x_n). \]
- We can have functions which are 0 everywhere except for one subbox at which this function grows to $1.1 \cdot \varepsilon$.
- On this subbox, the function is approximately quadratic.
- We have a bound $S$ on the second derivative.
7. Non-Quantum Lower Bound (cont-d)

- This function starts with 0 at a neighboring subbox.
- So, it cannot grow faster than $S \cdot x^2$ on this subbox.
- Thus, to reach a value larger than $\varepsilon$, we need to select $\delta$ for which $S \cdot (\delta/2)^2 = 1.1 \cdot \varepsilon$, i.e., the value $\delta \sim \varepsilon^{1/2}$.
- For this value $\delta$, we get $V/\delta^n \sim \varepsilon^{-(n/2)}$ subboxes:
  - if we do not explore some values of the optimized function at each of the subboxes,
  - we may miss the subbox that contains the largest value.
- Thus, we will not be able to localize the point at which the function attains its maximum.
- So, to locate the global maximum, we need at least as many computation steps as there are subboxes.
- So, we need at least time $\sim \varepsilon^{-(n/2)}$. 
8. This Lower Bound Is Reachable

- Let us show that there exists an algorithm that always locates the global maximum in time $\sim \varepsilon^{-\left(n/2\right)}$.
- Let us divide the box $B$ into subboxes of linear size $\delta$.
- For each subbox $b$, each of its sides has size $\leq \delta$.
- Thus, each component $x_i$ differs from the midpoint's $x^m = (x^m_1, \ldots, x^m_n)$ by no more than $\delta/2$:
  $$|\Delta x_i| \leq \delta/2, \text{ where } \Delta x_i \overset{\text{def}}{=} x_i - x^m_i.$$
- Thus, by using known formulas from calculus, we can conclude that for each point $x = (x_1, \ldots, x_n) \in b$:
  $$f(x_1, \ldots, x_n) = f(x^m_1 + \Delta x_1, \ldots, x^m_n + \Delta x_n) =$$
  $$f(x^m_1, \ldots, x^m_n) + \sum_{i=1}^{n} c_i \cdot \Delta x_i + \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} \cdot \Delta x_i \cdot \Delta x_j.$$
9. This Lower Bound Is Reachable (cont-d)

- Here $c_i \overset{\text{def}}{=} \frac{\partial f}{\partial x_i}(x_1^m, \ldots, x_n^m)$, and $c_{ij} \overset{\text{def}}{=} \frac{\partial^2 f}{\partial x_i \partial x_j}(\xi_1, \ldots, \xi_n)$ for some $\xi_1, \ldots, \xi_n) \in b$.

- We assumed that the function $f$ is twice continuously differentiable.

- So, all its second derivatives are continuous.

- Thus, there exists a general bound $S$ on all the values of all second derivatives: $|c_{ij}| \leq S$.

- Because of these bounds, the quadratic terms in the above formula are bounded by $n^2 \cdot S \cdot (\delta/2)^2 = O(\delta^2)$. 
10. These Estimations Lead to a Global Piece-Wise Linear Approximate Function

- By considering only linear terms on each subbox, we get an approximate piece-wise linear function $f \approx (x_1, \ldots, x_n)$.

- On each subbox $b$:

$$f \approx (x_1, \ldots, x_n) = f(x^m_1, \ldots, x^m_n) + \sum_{i=1}^{n} c_i \cdot \Delta x_i.$$ 

- For each $x = (x_1, \ldots, x_n)$, we have

$$|f(x_1, \ldots, x_n) - f \approx (x_1, \ldots, x_n)| \leq n^2 \cdot S \cdot (\delta/2)^2.$$
11. Optimizing the Approximate Function

- Let us find the point at which linear function $f \approx (x_1, \ldots, x_n)$ attains its maximum.

- On $[x_1^m - \delta/2, x_1^m + \delta/2] \times \ldots \times [x_n^m - \delta/2, x_n^m + \delta/2]$, as one can easily see:
  - the function $f \approx (x_1, \ldots, x_n)$ is increasing with respect to each $x_i$ when $c_i \geq 0$ and
  - the function $f \approx (x_1, \ldots, x_n)$ is decreasing with respect to $x_i$ if $c_i \leq 0$.

- Thus:
  - when $c_i \geq 0$, the maximum of the function $f \approx (x_1, \ldots, x_n)$ on this subbox is attained when $x_i = x_i^m + \delta/2$,
  - when $c_i \leq 0$, the maximum of the function $f \approx (x_1, \ldots, x_n)$ on this subbox is attained when $x_i = x_i^m - \delta/2$.

- We can combine both cases by saying that the maximum is attained when $x_i = x_i^m + \text{sign}(c_i) \cdot (\delta/2)$. 
12. Optimizing $f_{\approx}(x)$ (cont-d)

- Here $\text{sign}(x)$ is the sign of $x$ (i.e., 1 if $x \geq 0$ and $-1$ otherwise).

- We can:
  - repeat this procedure for each subbox,
  - find the corresponding largest value on each subbox, and then
  - find the largest of these values.

- This largest value is attained at a point $x^M = (x_1^M, \ldots, x_n^M)$.

- So, here is where $f_{\approx}(x_1, \ldots, x_n)$ attains its maximum.
13. Proof of Correctness

- Let us show that the point $x^M = (x^M_1, \ldots, x^M_n)$ is indeed a solution to the given optimization problem.
- Indeed, let $x^{\text{opt}} = (x^{\text{opt}}_1, \ldots, x^{\text{opt}}_n)$ be a point where the original function $f(x_1, \ldots, x_n)$ attains its maximum.
- Since $f_{\approx}(x)$ attains its maximum at $x^M$, we have
  $$f_{\approx}(x^M) \geq f_{\approx}(x) \text{ for all } x.$$ 
- In particular, $f_{\approx}(x^M_1, \ldots, x^M_n) \geq f_{\approx}(x^{\text{opt}}_1, \ldots, x^{\text{opt}}_n)$.
- The functions $f_{\approx}(x_1, \ldots, x_n)$ and $f(x_1, \ldots, x_n)$ are $\eta$-close, where $\eta \overset{\text{def}}{=} n^2 \cdot S \cdot (\delta/2)^2$.
- So, $f(x^M_1, \ldots, x^M_n) \geq f_{\approx}(x^M_1, \ldots, x^M_n) - \eta$ and
  $$f_{\approx}(x^{\text{opt}}_1, \ldots, x^{\text{opt}}_n) \geq f(x^{\text{opt}}_1, \ldots, x^{\text{opt}}_n) - \eta = M - \eta.$$
14. Proof of Correctness (cont-d)

- From these inequalities, we conclude that

\[
    f(x_1^M, \ldots, x_n^M) \geq f_\approx(x_1^M, \ldots, x_n^M) - \eta \geq f_\approx(x_1^{opt}, \ldots, x_n^{opt}) - \eta \geq (M - \eta) - \eta = M - 2\eta.
\]

- So, \( f(x_1^M, \ldots, x_n^M) \geq M - 2\eta. \)

- Thus, for \( \eta = \varepsilon / 2 \), we indeed get a solution to the original problem.
15. How Much Computation Time Do We Need

• To solve the original problem with a given $\varepsilon$, we need to select the value $\delta$ for which

$$2n^2 \cdot S \cdot (\delta/2)^2 = \varepsilon.$$  

• So, we need $\delta = c \cdot \varepsilon^{1/2}$, for an appropriate constant $c$.

• In this algorithm, we divide the whole box $B$ of volume $V$ into $V/\delta^n$ subboxes of linear size $\delta$.

• Since $\delta \sim \varepsilon^{1/2}$, the overall number of subboxes is proportional to $\varepsilon^{-n/2}$.

• On each subbox, the number of computational steps does not depend on $\varepsilon$.

• So, the overall computation time is proportional to the number of boxes, i.e.,

$$T = \text{const} \cdot \varepsilon^{-n/2}.$$

• We have bounded the function on a subbox.

• Similarly, we can find the bounds $F$ and $\overline{F}$ on $f(x_1, \ldots, x_n)$ over the whole box $B$.

• These bounds also bound the maximum $M$ of the function $f(x_1, \ldots, x_n)$: $M \in [F, \overline{F}]$.

• By selecting an appropriate $\delta \sim \varepsilon^{1/2}$, we can get an approximate function $f_{\approx}(x)$ which is $(\varepsilon/4)$-close to $f(x)$.

• Because of this closeness, the maximum $M_{\approx}$ of the approximate function is $(\varepsilon/2)$-close to the maximum $M$.

• Thus, $M_{\approx} \in [A_0, \overline{A}_0]$, where

$$A_0 \overset{\text{def}}{=} F - \varepsilon/2 \quad \text{and} \quad \overline{A}_0 \overset{\text{def}}{=} \overline{F} + \varepsilon/2.$$
17. Auxiliary Quantum Algorithm and Its Use

• For each $A$, Grover’s algorithm finds, in time $\sim \sqrt{N}$:
  – one of $N$ subboxes at which the maximum of $f_\approx(x)$ on this subbox is larger than or equal to $A$
  – or that there is no such subbox.

• Let us assume that we know an interval $[A, \overline{A}]$ that contains the maximum $M_\approx$ of $f_\approx$.

• Let’s use the above algorithm for $A = (A + \overline{A})/2$.

• If there is a subbox $b$ for which $f_\approx(x_0) \geq A$ for some $x_0 \in b$, then $M_\approx = \max_{x \in B} f_\approx(x) \geq f(x_0) \geq A$, so $M_\approx \in [A, \overline{A}]$.

• If no such subbox exists, then $f_\approx(x) \leq A$ for all $x$, so $M_\approx \leq A$ and $M_\approx \in [A, A]$.

• In both cases, we get a half-size interval containing $M_\approx$. 
18. **Main Algorithm: First Part**

- We start with the interval $[\underline{A}, \overline{A}] = [\underline{A}_0, \overline{A}_0]$ that contains the actual value $M_\approx$.

- At each iteration, we apply the above idea with 
  
  $$A = (\underline{A} + \overline{A})/2.$$ 

- As a result, we come up with a half-size interval containing $M_\approx$.

- In $k$ steps, we decrease the width of the interval $2^k$ times, to $2^{-k} \cdot (\overline{A} - \underline{A})$.

- In particular, in $k \approx \ln(\varepsilon)$, we can get an interval $[\underline{a}, \overline{a}]$ containing $M_\approx$ whose width is $\leq \varepsilon/4$: $\underline{a} \leq M_\approx \leq \overline{a}$. 
19. Main Algorithm: Second Part

- Since $a$ is $\leq$ the maximum $M_\approx$ of $f_\approx(x_1, \ldots, x_n)$, one of the values of this approximate function is indeed $\geq a$.

- The above auxiliary quantum algorithm will then find, in time $\sim \sqrt{N}$, a point $x_q = (x^q_1, \ldots, x^q_n)$ for which

$$f_\approx(x^q_1, \ldots, x^q_n) \geq a.$$
20. Proof of Correctness

• Let us prove that the resulting point \( x^q = (x^q_1, \ldots, x^q_n) \) indeed solves the original optimization problem.

• Indeed, by the very construction of this point, the value \( f \approx (x^q) \) is greater than or equal to \( a \).

• Since \( f \approx (x^q) \) cannot exceed the maximum value \( M \approx \) of \( f \approx (x) \), and \( M \approx \leq \bar{a} \), we conclude that \( f \approx (x^q) \leq \bar{a} \).

• Thus, both \( f \approx (x^q) \) and \( M \approx \) belong to the same interval \( [a, \bar{a}] \) of width \( \leq \varepsilon/4 \).

• So, the value \( f \approx (x^q) \) is \( (\varepsilon/4) \)-close to the maximum \( M \approx \).
21. Proof of Correctness (cont-d)

- In particular, this implies that
  \[ f_{\approx}(x_1^q, \ldots, x_n^q) \geq M_{\approx} - \varepsilon/4. \]

- Since \( f_{\approx}(x_1, \ldots, x_n) \) and \( f(x_1, \ldots, x_n) \) are \((\varepsilon/4)\)-close, their maximum values \( M_{\approx} \) and \( M \) are also \((\varepsilon/4)\)-close.

- In particular, this implies that \( M_{\approx} \geq M - \varepsilon/4 \), hence
  \[ f(x_1^q, \ldots, x_n^q) \geq M - \varepsilon/2. \]

- Since the functions are \((\varepsilon/4)\)-close, we conclude that
  \( f(x_1^q, \ldots, x_n^q) \geq f_{\approx}(x_1^q, \ldots, x_n^q) - \varepsilon/4 \) and thus, that
  \[ f(x_1^q, \ldots, x_n^q) \geq f_{\approx}(x_1^q, \ldots, x_n^q) - \varepsilon/4 \geq (M - \varepsilon/2) - \varepsilon/4 > M - \varepsilon. \]

- Thus, we indeed get the desired solution to the optimization problem.
22. What is the Computational Complexity of This Quantum Algorithm

- We need $\sim \ln(\varepsilon)$ iterations each of which requires time
  $$\sim \sqrt{N} \sim \sqrt{\varepsilon^{-\frac{n}{2}}} = \varepsilon^{-\frac{n}{4}}.$$  

- Thus, the overall computation time $T_q$ of this quantum algorithm is equal to $T_q \sim \varepsilon^{-\frac{n}{4}} \cdot \ln(\varepsilon)$.  

- We know that the computation time $T$ of the non-quantum algorithm is $T \sim \varepsilon^{-\frac{n}{2}}$; thus, $\varepsilon^{-\frac{n}{4}} \sim \sqrt{T}$.  

- Here, $\varepsilon \sim T^{-\frac{2}{n}}$, and thus, $\ln(\varepsilon) \sim \ln(T)$.  

- Thus, we conclude that  
  $$T_q \sim \sqrt{T} \cdot \ln(T).$$  

- The main result is thus proven.
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