Quantum Speed-Up of Estimating Partition Functions

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Content

- Partition Function, FPRAS and Simulated Annealing
- Classical Algorithm and Its Complexity
- Quantum Algorithm and the Speed-up
- Summary and Related Articles

Estimating Partition Functions

- let Ω be a set whose elements x correspond the states of some physical system
- let $E : \Omega \to \mathbb{R}$ denote the energy function, assigning each state x its energy $E(x)$
- given the desired (inverse) temperature β, the task is to estimate the partition function $Z(\beta)$

$$Z(\beta) = \sum_{x \in \Omega} e^{-\beta E(x)}$$

Computational Complexity

- the problem of estimating $Z(\beta)$ with high degree of accuracy for general $E : \Omega \to \mathbb{R}$ and high β is #P-hard (eg. 3-SAT with $E(x)$ as number of violated clauses.)

- $\Longrightarrow$ It is unlikely that there are efficient (classical and quantum) algorithms for this task

FPRAS

- we consider fully polynomial randomized approximation schemes (FPRAS)
- a FPRAS
  - outputs a random number $\hat{Z}$ satisfying

    $$\Pr\Big((1-\epsilon)Z(\beta) \leq \hat{Z} \leq (1+\epsilon)Z(\beta)\Big) \geq 3/4$$

    where $\epsilon \in (0,1)$ determines the desired accuracy
  - runs in time polynomial in problem size (that is $\log|\Omega|$) and $1/\epsilon$

Simulated Annealing

- choose a cooling schedule $\beta_0 < \beta_1 < \cdots < \beta_\ell$ with $\beta_0 = 0$ and $\beta_\ell = \beta$
- express the desired quantity as a telescoping product

$$Z(\beta) = \frac{Z(\beta_\ell)}{Z(\beta_{\ell-1})} \cdot \frac{Z(\beta_{\ell-1})}{Z(\beta_{\ell-2})} \cdots \frac{Z(\beta_1)}{Z(\beta_0)} \cdot Z(\beta_0)$$

- observe that $Z(\beta_0)$ is trivial since $Z(\beta_0) = |\Omega|$
- $\Rightarrow$ estimate the ratios $\alpha_i := Z(\beta_{i+1})/Z(\beta_i)$

Estimation via Boltzmann Sampling I

- denote by $\pi_i = \big(\pi_i(x) : x \in \Omega\big)$ the Boltzmann distribution at inverse temperature β_i

$$\pi_i(x) = \frac{e^{-\beta_i E(x)}}{Z(\beta_i)}$$

- assume we can sample from π_i
- assume we can find a short cooling schedule so that each ratio $\alpha_i := Z(\beta_{i+1})/Z(\beta_i)$ is bounded from below by a constant, say $1/2$
- $\Rightarrow$ by Chebyshev inequality it suffices to take $O(1/\epsilon^2)$ samples $\sim \pi_i$ to estimate α_i

Estimation via Boltzmann Sampling II

- let $X_i \sim \pi_i$ (that is $P(X_i = \sigma) = \pi_i(\sigma)$)
- let $\Delta\beta_i = \beta_{i+1} - \beta_i$
- define a new random variable

$$Y_i = e^{-\Delta\beta_i E(X_i)}$$

- the expected value $\mathbf{E}(Y_i)$ is equal to

$$\sum_{x\in\Omega} \pi_i(x) e^{-\Delta\beta_i E(x)} = \sum_{x\in\Omega} \frac{e^{-\beta_i E(x)}}{Z(\beta_i)} e^{(-\beta_{i+1}+\beta_i)E(x)} = \alpha_i$$

- $\Rightarrow Y_i$ is an unbiased estimator for α_i

Estimation via Boltzmann Sampling III

- draw $O(\ell/\epsilon^2)$ samples of X_i and compute the mean $\bar{Y}_i$
- $\Rightarrow$ the random variable $\bar{Y} = \bar{Y}_0 \bar{Y}_1 \cdots \bar{Y}_\ell$ satisfies

$$\Pr\Big((1-\epsilon)\alpha < \bar{Y} < (1+\epsilon)\alpha\Big) \geq 7/8$$

  where $\alpha = \alpha_0 \alpha_1 \cdots \alpha_\ell$

- $\Rightarrow$ the total number of samples is

$$O\Big(\ell^2/\epsilon^2\Big)$$

Sampling with Markov Chains

- in general, we are not able to sample directly from π_i
- for some $E : \Omega \to \mathbb{R}$, we can construct a Markov chain P_i such that
  - its stationary distribution is equal to π_i
  - its spectral gap δ is large
- $\Rightarrow$ we simulate

$$\tilde{O}(1/\delta)$$

steps of P_i to obtain one sample from $\tilde{\pi}_i$, which is sufficiently close to π_i

Quantum Walk

- the quantum walk $W(P_i)$ is a unitary such that its unique eigenvector with eigenvalue 1 is

$$|\pi_i\rangle = \sum_{x \in \Omega} \sqrt{\pi_i(x)}|x\rangle$$

- $|\pi_i\rangle$ is a coherent version of the limiting distribution π_i

Quadratic Relation

- the phase gap Δ of $W(P_i)$ is

$$\min\{|\varphi| : \ e^{i\varphi} \text{ is an eigenvalue of } W(P_i),\ e^{i\varphi} \neq 1\}$$

- the quadratic relation between the phase and spectral gaps

$$\Delta \geq \sqrt{\delta}$$

  is at the heart of quantum speed-ups of many search problems

- this makes it possible to realize the $2|\pi_i\rangle\langle\pi_i| - I$ by invoking $W(P_i)$ $O(\frac{1}{\sqrt{\delta}})$ times.

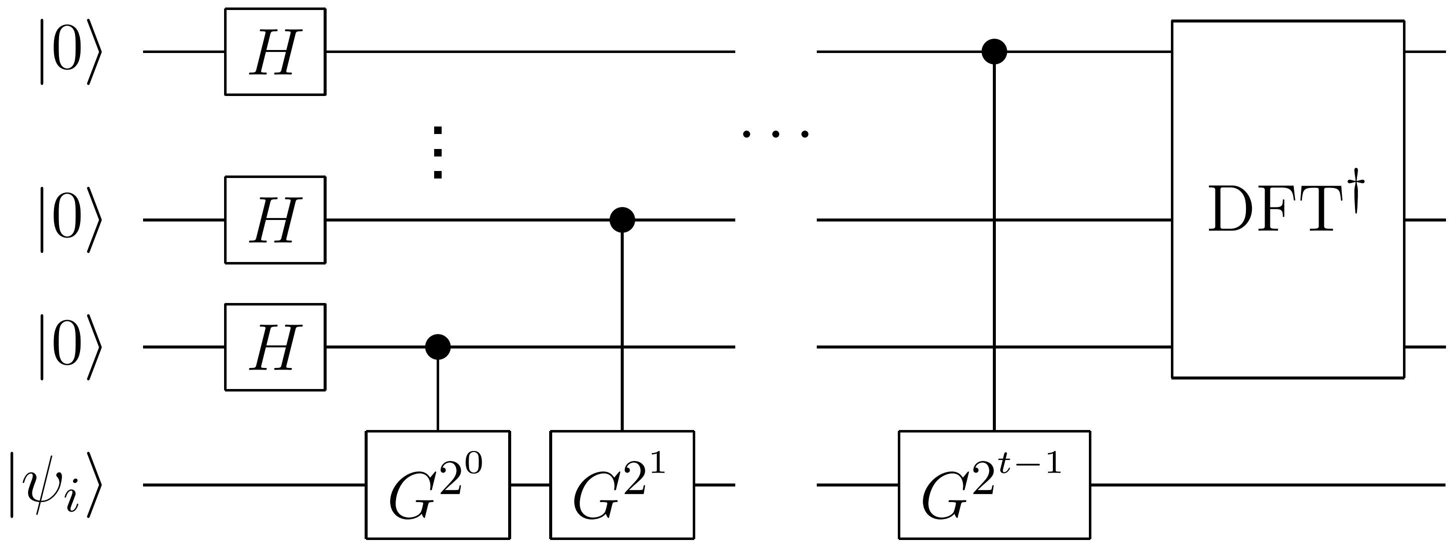
Structure of the Quantum Algorithm

$$|\pi_0\rangle \quad \boxed{\tilde{\alpha}_0}$$

$$|\pi_0\rangle \longrightarrow |\tilde{\pi}_1\rangle \quad \boxed{\tilde{\alpha}_1}$$

$$|\pi_0\rangle \longrightarrow |\tilde{\pi}_1\rangle \longrightarrow \cdots \longrightarrow |\tilde{\pi}_{\ell-1}\rangle \quad \boxed{\tilde{\alpha}_{\ell-1}}$$

Quantum Estimation of the Ratios



Preparation of Quantum Samples I

- the fact that the ratios α_i are bounded from below by $1/2$ implies

$$|\langle \pi_i | \pi_{i+1} \rangle|^2 \geq \frac{1}{2}$$

- $\Rightarrow$ we can drive $|\pi_i\rangle$ to $|\tilde{\pi}_{i+1}\rangle$ by applying $W(P_i)$ and $W(P_{i+1})$

$$\tilde{O}\Big(\frac{1}{\sqrt{\delta}}\Big)$$

  times

- this is based on Grover's $\frac{\pi}{3}$-fixed point search

Preparation of Quantum Samples II

- starting from $|\pi_0\rangle$ (uniform superposition), we can prepare any $|\tilde{\pi}_i\rangle$ by

$$|\pi_0\rangle \longrightarrow |\tilde{\pi}_1\rangle \longrightarrow \cdots \longrightarrow |\tilde{\pi}_i\rangle \longrightarrow \cdots \longrightarrow |\tilde{\pi}_{\ell-1}\rangle$$

- $\Rightarrow$ it suffices to apply operators in $\{W(P_k) : k = 0, \ldots, i\}$

$$\tilde{O}\Big(\frac{i}{\sqrt{\delta}}\Big)$$

  times

- $\Rightarrow$ the complexity of preparing $|\tilde{\pi}_0\rangle$, . . ., and $|\tilde{\pi}_{\ell-1}\rangle$ is

$$\tilde{O}\Big(\frac{\ell^2}{\sqrt{\delta}}\Big)$$

Quantum Estimation of the Ratios I

- let A_i be the observable

$$A_i = \sum_{x \in \Omega} e^{-\Delta\beta_i E(x)} |x\rangle\langle x|$$

- we have

$$\langle \pi_i | A_i | \pi_i \rangle = \alpha_i$$

where

$$|\pi_i\rangle = \sum_{x \in \Omega} \sqrt{\pi_i(x)} |x\rangle$$

Quantum Estimation of the Ratios II

- let

$$V_i := \sum_{x \in \Omega} |x\rangle\langle x| \otimes \begin{pmatrix} \sqrt{e^{-\Delta\beta_i E(x)}} & \sqrt{1 - e^{-\Delta\beta_i E(x)}} \\ -\sqrt{1 - e^{-\Delta\beta_i E(x)}} & \sqrt{e^{-\Delta\beta_i E(x)}} \end{pmatrix}$$

- let

$$|\psi_i\rangle = V_i\Big(|\pi_i\rangle \otimes |0\rangle\Big) \quad \text{and} \quad \Gamma := I \otimes |0\rangle\langle 0|$$

- $\Rightarrow$ we have

$$\begin{aligned} \langle\psi_i|\Gamma|\psi_i\rangle &= \langle\pi_i|A_i|\pi_i\rangle \\ &= \alpha_i \end{aligned}$$

Quantum Estimation of the Ratios III

- we obtain a random variable Q_i with

$$\Pr\left(\left(1-\frac{\epsilon}{2\ell}\right)\alpha_i \le Q_i \le \left(1+\frac{\epsilon}{2\ell}\right)\alpha_i\right) \ge 1-\frac{1}{8\ell}$$

  by applying quantum phase estimation to

$$G_i = \big(2|\psi_i\rangle\langle\psi_i| - I\big)\big(2\Gamma - I\big)$$

- to achieve the desired accuracy, we have to apply G_i

  $\tilde{O}\left(\frac{\ell}{\epsilon}\right)$ while G_i invokes $\tilde{O}(1/\sqrt{\delta})$ Walk operator $W(P_i)$.

Quantum Estimation of the Ratios IV

- consider the random variable $Q_0 Q_1 \cdots Q_{\ell-1}$
- $\Rightarrow$ we have

$$\Pr\Big((1-\epsilon)\alpha \leq Q \leq (1+\epsilon)\alpha\Big) \geq \frac{7}{8}$$

- the success probability decreases to $\geq 3/4$ due to imperfections ($|\tilde{\pi}_i\rangle$ and $2|\tilde{\pi}_i\rangle\langle\tilde{\pi}_i| - I$)
- to obtain the desired accuracy, it suffices to apply operators in $\{W(P_k) : k = 0, \ldots, \ell - 1\}$

$$O\Big(\frac{\ell^2}{\sqrt{\delta}\epsilon}\Big)$$

times

Summary: Quantum Speed-Up

- classical complexity

$$\tilde{O}\Big(\ell^2/(\delta\epsilon^2)\Big)$$

- quantum complexity

$$\tilde{O}\Big(\ell^2/(\sqrt{\delta}\epsilon)\Big)$$

- $1/\delta \rightarrow 1/\sqrt{\delta}$ is due to the quadratic relation between the spectral gaps of P_i and the phase gaps of the corresponding quantum walks $W(P_i)$
- $\epsilon^2 \rightarrow \epsilon$ is due to quantum estimation of expected values of observables

Future Research

- improving upon Chebyshev sampling on a quantum computer?
- quantum speed-up of
  - estimating permanents of matrices with non-negative entries?
  - quantum speed-up of estimating the volume of a convex polytope?
  - quantum speed-up of other classical approximation algorithms?
- estimating partition functions of quantum Hamiltonians

Related Articles

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