Quantum Techniques in Machine Learning 2023

Quantum Metropolis-Hastings algorithm with the target distribution calculated by quantum Monte Carlo integration

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Markov chain Monte Carlo method & Metropolis-Hastings algorithm

- Markov chain Monte Carlo method (MCMC)
  - sample from the *target distribution* P by generating a chain of samples $x_0 \to x_1 \to x_2 \to \cdots$ s.t. the distribution of x_i converges to P
  - often used for Bayesian inference (e.g. parameter optimization in machine learning)
- Metropolis-Hastings method (MH): a widely-used kind of MCMC
  - given the ith sample x_i, the $(i+1)$th one x_{i+1} is chosen as follows
    1. randomly draw a candidate $\tilde{x}_{i+1}$ from the *proposal distribution* $T(x_i,\cdot)$
    2. calculate the *acceptance ratio* $A(x_i, \tilde{x}_{i+1}) = \min\left\{1, \frac{P(\tilde{x}_{i+1})T(\tilde{x}_{i+1},x_i)}{P(x_i)T(x_i,\tilde{x}_{i+1})}\right\}$
    3. set $x_{i+1} = \tilde{x}_{i+1}$ with prob. $A(x_i, \tilde{x}_{i+1})$, or $x_{i+1} = x_i$ with prob. $1 - A(x_i, \tilde{x}_{i+1})$
- Convergence rate of MCMC
  - # of iterations for the chain to converge to P: $\tilde{O}(1/\Delta)$ ¶
    - ✓spectral gap $\Delta = 1 - |\lambda_1|$
      λ_1= (the eigenvalue of the transition matrix W with the 2nd largest modulus)

¶ in terms of total variation distance (Levin & Peres, “Markov chains and mixing times” (2017))

Quantum algorithm for MCMC

- Quantum simulated annealing (QSA)†
  - generates P-encoding state $|P\rangle := \sum_x \sqrt{P(x)}|x\rangle$ querying the *quantum walk operator* U $\tilde{O}(1/\sqrt{\Delta})$ time
    → **quadratic speedup** compared to classical MCMC $\tilde{O}(1/\Delta)$
- For MH, a concrete implementation of U is given¶
  - acts on a system of 2 registers R_S, R_M and 1 qubit R_C
  - $U = RV^\dagger B^\dagger SFBV$
    - ✓ $V|x\rangle_{R_S}|0\rangle_{R_M} = |x\rangle_{R_S}\sum_{\Delta x}\sqrt{T(x, x+\Delta x)}|\Delta x\rangle_{R_M}$ (Δx: possible move)
    - ✓ $B|x\rangle_{R_S}|\Delta x\rangle_{R_M}|\phi\rangle_{R_C} = |x\rangle_{R_S}|\Delta x\rangle_{R_M} \otimes \begin{pmatrix} \sqrt{1-A(x,x+\Delta x)} & -\sqrt{A(x,x+\Delta x)} \\ \sqrt{A(x,x+\Delta x)} & \sqrt{1-A(x,x+\Delta x)} \end{pmatrix}|\phi\rangle_{R_C}$
    - ✓ $F|x\rangle_{R_S}|\Delta x\rangle_{R_M}|0\rangle_{R_C} = |x\rangle_{R_S}|\Delta x\rangle_{R_M}|0\rangle_{R_C}, F|x\rangle_{R_S}|\Delta x\rangle_{R_M}|1\rangle_{R_C} = |x+\Delta x\rangle_{R_S}|\Delta x\rangle_{R_M}|1\rangle_{R_C}$
    - ✓ $S|\Delta x\rangle_{R_M}|0\rangle_{R_C} = |\Delta x\rangle_{R_M}|0\rangle_{R_C}, S|\Delta x\rangle_{R_M}|1\rangle_{R_C} = |-\Delta x\rangle_{R_M}|1\rangle_{R_C}$
    - ✓ $R = I_{R_S} \otimes \left(2|0\rangle\langle 0|_{R_M} \otimes |0\rangle\langle 0|_{R_C} - I_{R_M} \otimes I_{R_C}\right)$

† Harrow & Wei, SODA 2020 ¶ Lemieux et al., Quantum 4, 287 (2020)

Issue: target distribution calculated via summation of many terms

- e.g., optimization of the parameter x in a statistical model with a large data set $\mathcal{D}$ in the Bayesian approach
  - ➢ we want to optimize the posterior distribution of x:
    $P(x|\mathcal{D}) \propto P_0(x)P(\mathcal{D}|x)$ ($P_0(x)$: prior distribution)
    - ✓likelihood $P(\mathcal{D}|x) = \exp(L_{\mathcal{D}}(x))$
      log-likelihood $L_{\mathcal{D}}(x) = \frac{1}{M}\sum_{i=0}^{M-1} \ell_i(x), M \gg 1$ ← **sum of many terms**
      $\ell_i(x)$: contribution from the ith data point in $\mathcal{D}$

- **Can we run MH with speeding up the summation by a quantum algorithm?**

Our idea: speed up the summation by QMCI

- We use **quantum Monte Carlo integration (QMCI)**† for $L_{\mathcal{D}}(x) = \frac{1}{M}\sum_{i=0}^{M-1} \ell_i(x)$, and incorporate it into QSA

- QMCI
  - a quantum algorithm to calculate an expectation of a random variable (and a sum as a special case)
  - calculate $L_{\mathcal{D}}(x) = \frac{1}{M}\sum_{i=0}^{M-1} \ell_i(x)$ querying the oracle O_ℓ to compute ℓ_i
    $O_\ell|x\rangle|i\rangle|0\rangle = O_\ell|x\rangle|i\rangle|\ell_i(x)\rangle$
  - for accuracy ϵ, the query number is $\tilde{O}(\sigma/\epsilon)$
    - ✓ σ^2: the variance of the terms ℓ_i
      $\sigma^2 \coloneqq \max_x \frac{1}{M}\sum_{i=0}^{M-1} \ell_i^2(x) - \left(\frac{1}{M}\sum_{i=0}^{M-1} \ell_i(x)\right)^2$
    - ✓ **quadratic speedup** compared to classical Monte Carlo integration: $\tilde{O}(\sigma^2/\epsilon^2)$

† Montanaro, Proc. R. Soc. A, 471(2181):20150301 (2015)

Drawback of using QMCI

- QMCI outputs $L_{\mathcal{D}}$ with an **error**
  → error in the acceptance ratio A
  → the chain converges to the distribution P' different from the target P

➢ If we use A' s.t. $\max_{x,y}|A(x,y) - A'(x,y)| \leq \epsilon$,
$\|P - P'\|_{TV} = \tilde{O}(\epsilon/\Delta)$ ¶
(TV: total variation distance)

⬇

➢ For $\|P' - P\|_{\mathrm{TV}} \leq \epsilon$, it is sufficient that the error in $L_{\mathcal{D}}$ is $\tilde{O}(\epsilon\Delta)$

⬇

➢ query complexity in QMCI: $\tilde{O}(\sigma/\epsilon\Delta)$

¶ Alquier et al., Statistics and Computing 26, 29 (2016)

Result 1: Generating $|P\rangle$ by QSA with $L_{\mathcal{D}}$ calculated by QMCI

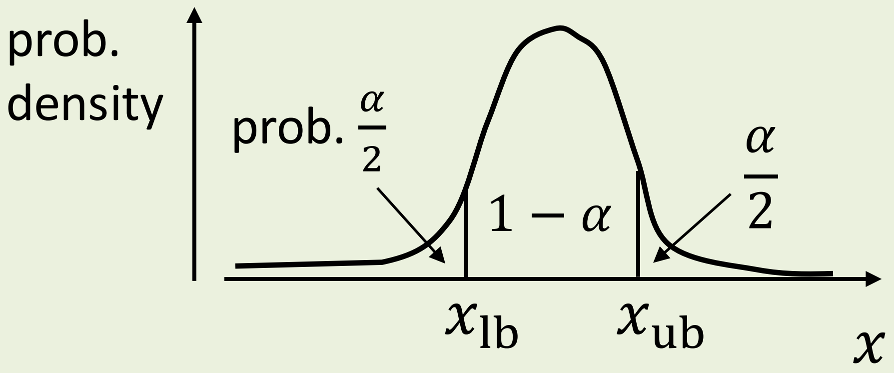
- Theorem (informal)
  - Suppose that we are given the oracle O_ℓ to compute ℓ_i.
    There is a quantum algorithm that outputs an ϵ-approximation of $|P\rangle := \sum_x \sqrt{P(x)}|x\rangle$, making $\tilde{O}\left(\sigma/\epsilon\Delta^{3/2}\right)$ queries to O_ℓ.

- In the *exact QSA*, in which $L_{\mathcal{D}} = \frac{1}{M}\sum_{i=0}^{M-1} \ell_i(x)$ is calculated as the definition (by M-time iterations of calculating $\ell_i(x)$ and adding it), the query number is $\tilde{O}\left(M/\Delta^{1/2}\right)$
  → QMCI improves the scaling on M, the number of terms, in compensation for ϵ, Δ

Estimation of the credible interval

- QSA outputs $|P\rangle$, but we want not a quantum state but some statistics on P as classical data

- Typical quantity of interest: credible interval (CI) of a parameter in a statistical model
  - $100(1-\alpha)\%$ CI for x:
    $[x_{\rm lb}, x_{\rm ub}]$ s.t. $P(x < x_{\rm lb}) = \frac{\alpha}{2}, P(x_{\rm ub} < x) = \frac{\alpha}{2}$



- Given the oracle to generate $|P\rangle$ by QSA, we can estimate $x_{\rm lb}, x_{\rm ub}$ as follows
  - We can calculate the cumulative distribution function (CDF) $\Phi(a) := P(x < a)$ as $\Phi(a) = E_P[\mathbf{1}_{x<a}] = \sum_x \mathbf{1}_{x<a} P(x)$, the expectation of the indicator function $\mathbf{1}_{x<a}$ in P, by QMCI
  - Calculating $\Phi(a)$ like this, we find $x_{\rm lb}, x_{\rm ub}$ by bisection (or other root-finding methods)

Result 2: CI estimation by QSA with QMCI

- Theorem (informal)
  - Suppose that we are given the oracle O_ℓ to compute ℓ_i.
    There is a quantum algorithm that outputs estimates on $x_{\mathrm{lb}}, x_{\mathrm{ub}}$ with accuracy ϵ (in terms of the CDF), making $\tilde{O}\left(\sigma/\epsilon^2\Delta^{3/2}\right)$ queries to O_ℓ.

- Based on the exact QSA, the query number is $\tilde{O}\left(M/\epsilon\Delta^{1/2}\right)$
  → QMCI improves the scaling on M, the number of terms, in compensation for ϵ, Δ

When QSA with QMCI is beneficial: σ sublinear w.r.t. M

- We defined $L_{\mathcal{D}}(x)=\frac{1}{M}\sum_{i=0}^{M-1}\ell_i(x)$

  → Note that the prefactor $1/M$, which does not always exist

  ➢ e.g., in the model parameter estimation with M independent data points, $L_{\mathcal{D}}(x)=\sum_{i=0}^{M-1}\ell_i(x)$ with ℓ_i not depending on M

- By redefining $\ell_i(x)\rightarrow M\ell_i(x)$, we can write $L_{\mathcal{D}}$ in the form $L_{\mathcal{D}}(x)=\frac{1}{M}\sum_{i=0}^{M-1}\ell_i(x)$, but this leads to $\sigma=O(M)$, which causes the advantage of QSA with QMCI to disappear

  ➢ Complexity of generating $|P\rangle$: $\tilde{O}\left(\sigma/\epsilon\Delta^{3/2}\right)=\tilde{O}\left(M/\epsilon\Delta^{3/2}\right)$

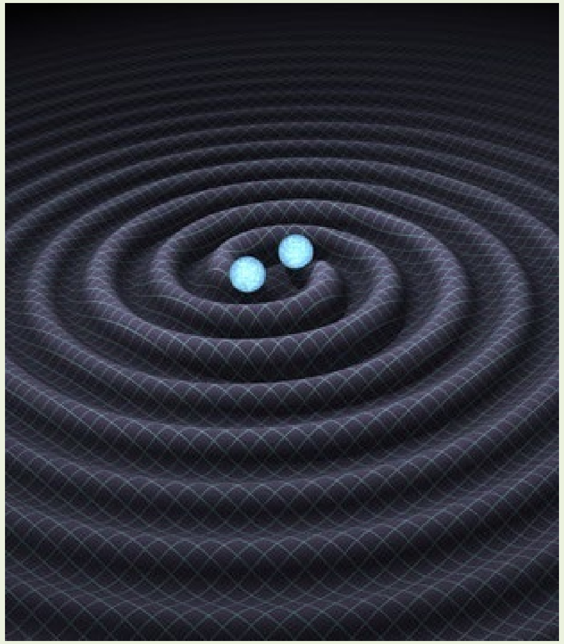
    → compared to the exact QSA ($\tilde{O}\left(M/\Delta^{1/2}\right)$), the scaling on M is same and those on ϵ,Δ are worse

- QSA with QMCI can be beneficial if **σ scales on M sublinearly**

  → e.g. **parameter estimation in a gravitational wave detection experiment**

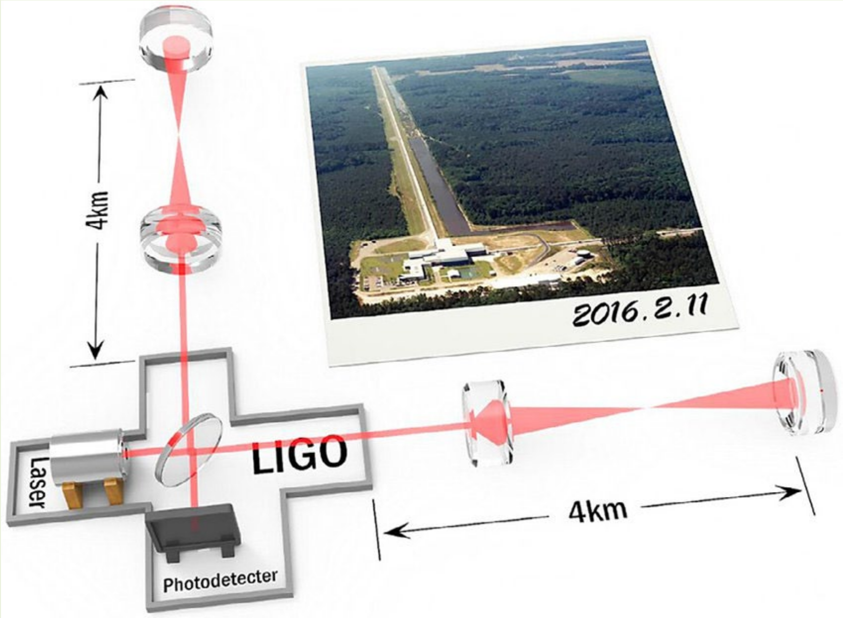
Gravitational wave

- Gravitational wave (GW)
  - wave of spacetime distortion caused by an extreme astrophysical event such as a merger of black holes (BHs)
  - detected by laser interferometers such as LIGO in US



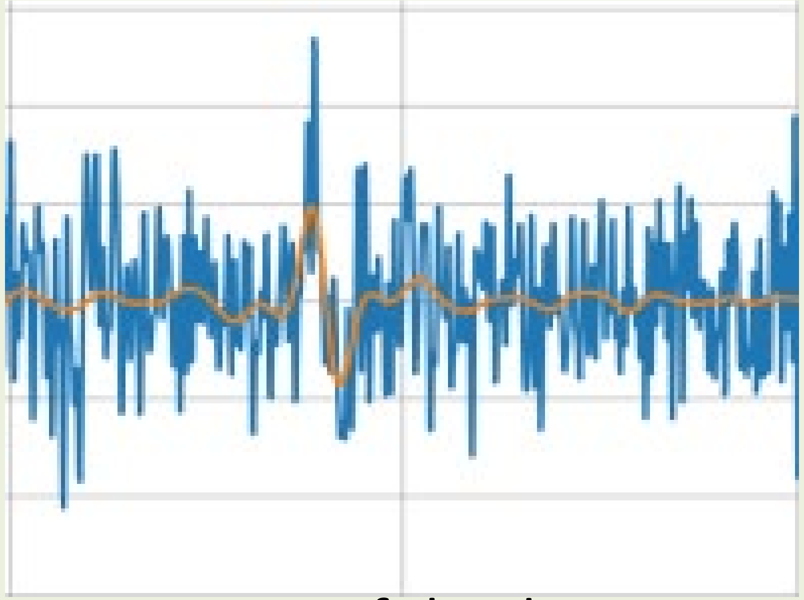
GW from BH merger

www.ligo.caltech.edu



Laser interferometer

Zuo+., Opt. Lasers Eng. 135, 106187 (2020)



output of the detector
(noise ≫ GW signal)

Morras+, Phys. Dark Universe 35, 100932 (2022)

Figures are for illustration purposes.

GW parameter estimation by QSA with QMCI

- We estimate GW parameters (e.g. BH's mass) from the signal in the detector output $s(t)$
  - If we have $s(t)$ as M-point time-series data with interval Δt,

$$L_{\mathcal{D}}(x) = \frac{1}{M/2}\sum_{i=1}^{M/2-1} \ell_i(x)\,, \ell_i(x) = \mathrm{Re}\left(\frac{4\tilde{h}^*(f_i,x)\tilde{s}(f_i)}{S_n(f_i)\Delta\mathrm{t}}\right) \text{¶}$$

    - ✓ ℓ_i: contribution from the Fourier mode with frequency $f_i = i/M\Delta t$
    - ✓ $\tilde{h}(f,x)$: Fourier-transformed theoretical waveform of GW depending on parameters x
    - ✓ $\tilde{s}$: Fourier-transf. of s, S_n: noise power spectrum
  - In this case, $\sigma = O(\sqrt{M})$, so QSA with QMCI can be beneficial
    - ✓ $\sigma = O(\sqrt{M})$ is due to the situation that random noise dominates over the GW signal in the detector output
- QSA with QMCI estimates the CI of a GW parameter with $\tilde{O}(M^{1/2}/\Delta^{3/2}\epsilon^2)$ queries to O_ℓ

¶ Some terms omitted.

Summary

- MCMC, especially MH is a widely used technique, e.g. Bayesian inference including parameter optimization in machine learning.
- QSA provides quadratic speedup with respect to spectral gap Δ compared with classical MH.
- We focused on another point, calculation of the log-likelihood $L_{\mathcal{D}}$ as a sum of many terms. We proposed speeding up the summation by QMCI and incorporated it into QSA.
- We consider not only generating the quantum state $|P\rangle$ but also extracting a quantity of interest, a credible interval.
- We present GW parameter estimation as an example where QSA with QMCI is beneficial.

- Summary of query complexity

Task	QSA with QMCI	Exact QSA	Classical MH
Generating $\|P\rangle$	$\tilde{O}(\sigma/\Delta^{3/2}\epsilon)$	$\tilde{O}(M/\Delta^{1/2})$	N/A
CI estimation (general)	$\tilde{O}(\sigma/\Delta^{3/2}\epsilon^2)$	$\tilde{O}(M/\Delta^{1/2}\epsilon)$	$\tilde{O}(M/\Delta\epsilon^2)$
CI estimation (GW)	$\tilde{O}(M^{1/2}/\Delta^{3/2}\epsilon^2)$	$\tilde{O}(M/\Delta^{1/2}\epsilon)$	$\tilde{O}(M/\Delta\epsilon^2)$