Quantum Speedups for Multiproposal MCMC

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ABSTRACT

Multiproposal Markov chain Monte Carlo (MCMC) algorithms choose from multiple proposals to generate their next chain step in order to sample from challenging target distributions more efficiently. However, on classical machines, these algorithms require O(P) target evaluations for each Markov chain step when choosing from P proposals. Recent work demonstrates the possibility of quadratic quantum speedups for one such multiproposal MCMC algorithm. After generating P proposals, this quantum parallel MCMC (QPMCMC) algorithm requires only O(P) target evaluations at each step, outperforming its classical counterpart. However, generating P proposals using classical computers still requires time complexity O(P), resulting in the overall complexity of QPMCMC remaining O(P). Here, we present a new, faster quantum multiproposal MCMC strategy, QPMCMC2. With a specially designed Tjelmeland distribution that generates proposals close to the input state, QPMCMC2 requires only O(1) target evaluations and Olog(P) qubits when computing over a large number of proposals P. Unlike its slower predecessor, the QPMCMC2 Markov kernel (1) maintains detailed balance exactly and (2) is fully explicit for a large class of graphical models. We demonstrate this flexibility by applying QPMCMC2 to novel Ising-type models built on bacterial evolutionary networks and obtain significant speedups for Bayesian ancestral trait reconstruction for 248 observed salmonella bacteria.

Keywords: Bayesian phylogenetics; MCMC; Quantum algorithms; Ising models

A Derivative-Free Approach for Parameter Inference in Hidden Quantum Markov Models

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ABSTRACT

Hidden Quantum Markov Models (HQMMs) provide a quantum-inspired framework for modeling complex sequential data, offering greater expressive power than classical Hidden Markov Models (HMMs). Existing learning algorithms for HQMMs typically rely on gradient-based optimization of the log-likelihood function, which can be computationally intensive and sensitive to local minima.

In this work, we propose a new and general method for inferring HQMM parameters that avoids the computation of derivatives of the log-likelihood. Our approach is broadly applicable to HQMMs with arbitrary Kraus operator structures and enables learning in settings where differentiability is difficult to guarantee or gradient computation is costly. We validate the proposed algorithm on synthetic datasets, demonstrating that it can successfully recover HQMM parameters and outperforms baseline methods in both accuracy and computational efficiency.

Keywords: Quantum computing; Hidden Markov Models; Sequential Data Modeling; Parameter Inference; Derivative-Free Optimization

Quantum Computations of Partial Differential Equations and Related Problems

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ABSTRACT

Quantum computers are designed based on quantum mechanics principle, they are most suitable to solve the Schrodinger equation, and linear PDEs (and ODEs) evolved by unitary operators. It is important to explore whether other problems in scientific computing, such as ODEs, PDEs, and linear algebra that arise in both classical and quantum systems which are not unitary evolution, can be handled by quantum computers.

We will present a systematic way to develop quantum simulation algorithms for general differential equations. Our basic framework is dimension lifting, that transfers non-autonomous ODEs/PDEs systems to autonomous ones, nonlinear PDEs to linear ones, and linear ones to Schrodinger type PDEs—coined “Schrodingerization”—with unitary evolutions. Our formulation allows both qubit and qumode (continuous-variable) formulations, and their hybridizations, and provides the foundation for analog quantum computing which are easier to realize in the near term. We will also present dimension lifting techniques for quantum simulation of stochastic DEs and PDEs with fractional derivatives, and quantum machine learning. A quantum simulation software—“UnitaryLab”—will also be introduced.

Keywords: quantum algorithms, Schrodingerization, partial differential equations, analog quantum computing, dimension lifting

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Adaptive Circuit Learning of Born Machine: Towards Realization of Amplitude Embedding and Quantum Data Loading

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ABSTRACT

Quantum data loading plays a central role in quantum algorithms and quantum information processing. Many quantum algorithms hinge on the ability to prepare arbitrary superposition states as a subroutine, with claims of exponential speedups often predicated on access to an efficient data-loading oracle. In practice, constructing a circuit to prepare a generic n-qubit quantum state typically demands computational efforts scaling as $O(2^n)$, posing a significant challenge for quantum algorithms to outperform their classical counterparts. To address this critical issue, various hybrid quantum–classical approaches have been proposed. However, many of these solutions favor simplistic circuit architectures, which are susceptible to substantial optimization challenges. In this study, we harness quantum circuits as Born machines to generate probability distributions. Drawing inspiration from methods used to investigate electronic structures in quantum chemistry and condensed matter physics, we propose a framework called Adaptive Circuit Learning of Born Machine, which dynamically expands the ansatz circuit. Our algorithm is designed to selectively integrate two-qubit entangled gates that best capture the intricate entanglement present within the target state. Empirical experiments underscore the efficacy of our approach in encoding real-world data through amplitude embedding, demonstrating not only compliance with but also enhancement over the performance benchmarks set by prior research.

Keywords: quantum data loading; born machine; quantum machine learning; amplitude encoding