

A Quantum-Quantum Metropolis Algorithm (Q²MA)

Background information

The classical Metropolis algorithm is an efficient way of sampling the Markov chain for producing an equilibrium distribution, e.g. spin model. The efficiency of a Markov chain is mostly determined by the eigenvalue gap Δ of the transition matrix M ; typically it goes as $1/\delta$.

Some years ago, Szegedy¹ pointed out that it is possible to make a quadratic quantum speedup for any classical Markov chain, and make the running time goes as $1/\sqrt{\delta}$. This leads to some interest² in employing Szegedy's method to prepare thermal states of classical systems.

On the other hand, to extend the Metropolis algorithm to the quantum domain is an interesting problem. Terhal and DiVincenzo³ attempted this problem in 2000. However, the method they described would not be efficient in the general case, as the update rule consists of too many energy non-local transitions. Recently, an improvement⁴ has been made; this basically introduces a method to allow random local unitary operators in the update rule. It is true that quantum Hamiltonians are now included in the Metropolis method. However, the underlying Markov chain is still classical. In other words, the scaling of this method still goes as $1/\delta$.

In this work, we combine the best of the both worlds; namely, a Metropolis algorithm which can deal with quantum Hamiltonians and is benefited by a quantum speedup from the Szegedy method. The scaling goes as $1/\sqrt{\delta}$. This result completes the picture of the generalization of the classical Metropolis methods to the quantum domain. Furthermore, the application of the Metropolis method for quantum Hamiltonian can be considered as a special case of quantum map (operation), it may be possible that the results presented here could be generalized to allow quantum speedup for a much broader class of quantum maps.

Basic Idea of the Metropolis method

Instead of showing the results of the full quantum version of the paper, I shall illustrate the key results by considering a classical version of it. At the same time, we

¹ M. Szegedy, Proceedings of the 45th IEEE Symposium on Foundations of Computer Science (2004), p. 32.

² R. Somma, S. Boixo, H. Barnum, and E. Knill, Phys. Rev. Lett. 101, 130504 (2008); P. Wocjan and A. Abeyesinghe, Phys. Rev. A 78, 042336 (2008).

³ B. M. Terhal and D. P. DiVincenzo, Phys. Rev. A 61, 022301 (2000).

⁴ K. Temme, T.J. Osborne, K.G. Vollbrecht, D. Poulin, and F. Verstraete, arXiv:0911.3635.

take this chance to review the basic idea of the Metropolis method. As example, we consider an Ising spin model. I shall describe it in a way that would make sense of using quantum computer to implement it.

Step 1: Start with a certain spin configuration $|x\rangle$.

Step 2: Copy the information of the state $|x\rangle$, i.e. $|x\rangle|0\rangle \rightarrow |x\rangle|x\rangle$

Step 3: Then flip the spin configuration in some way, i.e. $|x\rangle|x\rangle \rightarrow |x\rangle(K|x\rangle)$, here K is Pauli X matrix. We call this new configuration $|y\rangle \equiv K|x\rangle$.

Step 4: We compare two configuration, before and after the "kick"; then accept the move according to a probability distribution $z_{xy} = \min\left\{1, e^{-\beta(E_y - E_x)}\right\}$.

This is the basic idea of the Metropolis method. In the language of quantum computer, step 4 can be implemented by including an extra qubit, and rotated conditionally by some angle determined by the energies of the two spin configurations, i.e., $|0\rangle \rightarrow \sqrt{z_{xy}}|0\rangle + \sqrt{1-z_{xy}}|1\rangle$. Then, we apply a controlled SWAP and get:

$$U_x |x\rangle|x\rangle|0\rangle = \sqrt{z_{xy}} |x\rangle|y\rangle|0\rangle + \sqrt{1-z_{xy}} |y\rangle|x\rangle|1\rangle.$$

Here U_x summarizes the procedure. If now we keep the state of the first qubit and trace out the other qubits. Then, we indeed can get a mixed state, which is equivalent to the Metropolis method. From this point of view, it may now become not so surprising that U_x is somehow connected to the Metropolis transition matrix M in someway. Continue working with it along the line of Szegedy's method (see the paper), one can find that the energy gap of a matrix associated with U_x is larger than that of M . This is the original of the quantum speedup.

To generalize the method above to the quantum case, one may attempt to change

$$|x\rangle \rightarrow |\phi_x\rangle$$

to an eigenstate $|\phi_x\rangle$ of a quantum Hamiltonian. The key obstacle for generalizing the method described above is the no-cloning theorem, that in general the operation

$$|\phi_x\rangle|0\rangle \rightarrow |\phi_x\rangle|\phi_x\rangle \quad (\text{no !})$$

is not allowed if we do not know anything about $|\phi_x\rangle$. However, there is one trick this paper relies on. If we start with the maximally entangled state $\sum_x |x\rangle$, we can turn it into $\sum_x |x\rangle|x\rangle$ easily (e.g. by bit-by-bit controlled not), as $|x\rangle$ is just the computational basis. Now we formally insert an identity written as $I = \sum_i |\phi_i\rangle\langle\phi_i|$, then we have the following state: $\sum_i |\phi_i\rangle|\tilde{\phi}_i\rangle$, where $|\tilde{\phi}_i\rangle = \sum_x a_i^*(x)|x\rangle$ is the time-reversal counterpart of $|\phi_i\rangle \equiv \sum_x a_i(x)|x\rangle$. The expansion coefficients are complex conjugate of each other, and they have the same eigenvalue spectrum: $H|\phi_i\rangle = E_i|\phi_i\rangle$ and $H^*|\tilde{\phi}_i\rangle = E_i|\tilde{\phi}_i\rangle$. These pairs of states are therefore correlated, avoiding the restriction of quantum cloning. The basic idea of the paper is to take the initial state as $\sum_i |\phi_i\rangle|\tilde{\phi}_i\rangle$ (infinite temperature state), then we can work in the basis $|\phi_i\rangle|\tilde{\phi}_i\rangle$ and follow the Metropolis method (similar to the one described above), and obtain the thermal state in any temperature using quantum simulation annealing.

Summary

To summarize, in this work, we describe a revised version of the quantum Metropolis algorithm which extends Szegedy's method of classical Markov-chain quantization to the quantum domain, and provides a quadratic quantum speedup $1/\sqrt{\delta}$ in the gap δ of the transition matrix M . The restriction encountered by the previous version of the quantum Metropolis algorithm is mostly due to the no-cloning theorem, where the required information, such as the associated eigenvalue, of an eigenstate cannot be retrieved after the proposed move in the Metropolis step. We relax this restriction by adopting a dual representation where the set of basis states consists of pairs of eigenstates related by the time-reversal operation. This result completes the picture of the generalization of the classical Metropolis method to the quantum domain. Furthermore, the application of the Metropolis method for quantum Hamiltonian can be considered as a special case of quantum map (operation), it may be possible that the results presented here could be generalized to allow quantum speedup for a much broader class of quantum maps.