Relation of classical non-equilibrium dynamics and quantum annealing

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Abstract. Non-equilibrium dynamics of the Ising model is a classical stochastic process whereas quantum mechanics has no stochastic elements in the classical sense. Nevertheless, it has been known that there exists a close formal relationship between these two processes. We reformulate this relationship and use it to compare the efficiency of simulated annealing that uses classical stochastic processes and quantum annealing to solve combinatorial optimization problems. It is shown that classical dynamics can be efficiently simulated by quantum-mechanical processes whereas the converse is not necessarily true. This may imply that quantum annealing may be regarded as a more powerful tool than simulated annealing for optimization problems.

1. Introduction
Quantum annealing (QA) is a metaheuristic for combinatorial optimization problems. In the words of physics, the task is to find the ground state of the Ising model with generally complicated interactions [1, 2, 3, 4]. QA uses quantum fluctuations realized by transverse fields to search for the solution in the phase space. A restricted version of QA is adiabatic quantum computation, in which the system is supposed to follow the instantaneous ground state of the time-dependent Schrödinger equation [5]. QA may be regarded as the quantum-mechanical alternative to simulated annealing (SA) [6, 7], in which classical thermal fluctuations play the role of quantum fluctuations in QA. It is an interesting problem how QA can be better (or worse) than SA.

Recent years have observed high activities in this area, most of which indicate some kind of supremacy of QA over SA [1, 2, 3, 8]. Experimental approaches have also become available using the D-Wave machine [9]-[26]. Experimental data suggest that quantum effects indeed play roles at least to some extent.

Pioneering examples of numerical data, obtained from direct numerical integration of the Schrödinger equation and quantum Monte Carlo simulations, are found in the thesis of Kadowaki [8]. It has been found that the probability of the system being in the true ground state is larger in QA than in SA for spin glass cases and travelling salesman problems. It has also been shown that the achieved values of the final energy are lower in QA than in SA.

From the analytical side, theorems have been proven that give a sufficient condition for the time dependence of the strength of quantum fluctuations, i.e. the annealing schedule, such that the system reaches the ground state in the infinite-time limit [27, 28, 29, 30]. The resulting condition turns out to give a faster reduction of the control parameter in QA than in SA. It should nevertheless be remembered that this result does not mean that a given difficult problem...
can be solved efficiently by the quantum method. Theoretical supremacy of QA is usually quantitative, not qualitative, as far as the sufficient condition for the worst case is concerned.

One of the interesting questions is whether or not QA can be efficiently simulated on a classical computer. The above-mentioned sufficient condition indicates that the amplitude of the transverse field should be reduced as a function of time in the same manner in the natural Schrödinger dynamics and in the master equation dynamics corresponding to quantum Monte Carlo simulations [27, 28, 29]. This is a surprising result because the Schrödinger dynamics is completely different from the classical stochastic dynamics of Monte Carlo processes. The result may be understood to suggest that QA can be efficiently simulated on a classical computer. We should, however, be very careful because, first, quantum Monte Carlo operates at low but finite temperatures whereas the Schrödinger dynamics is a zero-temperature process. Second, quantum Monte Carlo is a stochastic sampling of the classical master equation. Directly solving the master equation consumes an exponential amount of time and memory on a classical computer, which is the same situation as in solving the Schrödinger equation directly on a classical computer.

In the present paper, we try to shed some light on this problem. Following [31], we show that an ingenious mapping between classical stochastic dynamics and a quantum system allows us to derive a conclusion that simulated annealing may be efficiently simulated by quantum annealing but the converse is not necessarily true.

2. Classical to quantum mapping
Let us first consider the classical dynamics of the Ising model described by the Hamiltonian $H_0(\sigma)$, where $\sigma$ stands for the set of $N$ Ising spins, $\sigma = \{\sigma_1, \sigma_2, \cdots, \sigma_N\}$. We have added a subscript 0 to the Hamiltonian to distinguish this classical Ising Hamiltonian from the quantum Hamiltonian defined later. The master equation for the probability $P_\sigma(t)$ that the system is in the state $\sigma$

$$\frac{dP_\sigma(t)}{dt} = \sum_\sigma W_{\sigma\sigma'} P_{\sigma'}(t),$$

(1)

where $W_{\sigma\sigma'}$ denotes an element of the transition matrix, defines the classical stochastic dynamics. The transition probability is a function of the temperature, which is implicit in the above notation. The temperature is fixed for the moment. The transition matrix has non-positive right eigenvalues

$$W_\psi^{(R,n)} = -\lambda_n \psi^{(R,n)}$$

(2)

with $\lambda_0 = 0$ and $0 > -\lambda_1 > -\lambda_2 > \cdots$. The leading eigenvector $\psi^{(R,0)}$ corresponds to the equilibrium state, and other eigenvectors represent relaxing modes. The solution to the master equation (1) has a general expression as

$$P_\sigma(t) = P_\sigma^{eq} + a_\sigma^{(1)} e^{-\lambda_1 t} + a_\sigma^{(2)} e^{-\lambda_2 t} + \cdots,$$

(3)

where $P_\sigma^{eq}$ is the equilibrium Gibbs-Boltzmann distribution. This expression makes it clear that the relaxation time toward equilibrium is the inverse of the leading non-vanishing eigenvalue,

$$\tau_{relax} = \frac{1}{\lambda_1}.$$  

(4)

The relaxation time diverges at a transition point $T = T_c$. If the transition is of second order, the relaxation time at $T = T_c$ diverges polynomially as the system size $N$ increases,

$$\tau_{relax} \left( = \frac{1}{\lambda_1} \right) \propto N^a \, (a > 0),$$

(5)
whereas the divergence is usually exponential at a first-order transition,
\[ \tau_{\text{relax}} \left( = \frac{1}{\lambda_1} \right) \propto e^{bN} \ (b > 0). \] (6)

This means that the energy gap between the leading eigenvalue \( \lambda_0 = 0 \) and the next eigenvalue \( \lambda_1 \) closes polynomially at a second-order transition point and exponentially at a first-order transition.

If we define a \( 2^N \times 2^N \) matrix \( H \) with element
\[ H_{\sigma\sigma'} = -e^{\beta H_0(\sigma)}/2 W_{\sigma\sigma'} e^{-\beta H_0(\sigma')}/2, \] (7)
where \( \beta \) is the inverse temperature, then the detailed balance condition \( W_{\sigma\sigma'} P_{\sigma'}^{\text{eq}} = W_{\sigma'\sigma} P_{\sigma}^{\text{eq}} \) imposed on the transition matrix guarantees that \( H \) is a symmetric matrix,
\[ H_{\sigma\sigma'} = H_{\sigma'\sigma}. \] (8)

Since all matrix elements of \( H \) are real, this is a Hermitian matrix and thus can be regarded as the Hamiltonian of a quantum system.

The Hamiltonian \( H \) shares the eigenstates and eigenvalues with \( W \), up to trivial factors,
\[ H\phi^{(n)} = \lambda_n \phi^{(n)}, \ \phi^{(n)} = e^{\beta H_0/2} \psi^{(R,n)} \] (9)
as can be verified from the definition (7). Since the energy gap between the ground and first excited states \( \Delta = \lambda_1 \) is common to both systems (the classical dynamical system and the quantum system), these two systems share the existence and properties of a phase transition. In particular, the energy gap of the quantum system closes polynomially as a function of the system size at a second-order quantum transition and exponentially at a first-order quantum transition if the same is true for the classical case.

It is to be noticed that this classical-to-quantum mapping preserves the spatial dimension of the system. It is also important to remember that the definition (7) leads to short-range interactions in \( H \) if the same is true for \( H_0 \) as can be verified from the definition (7). A simple example is the one-dimensional ferromagnetic Ising model
\[ H_0(\sigma) = -\sum_j \sigma_j \sigma_{j+1}, \] (10)
from which the following quantum Hamiltonian is derived under the heat-bath dynamics [31],
\[ H = -\frac{1}{2} \sum_j \sigma_j^z \sigma_{j+1}^z - \frac{1}{2 \cosh \beta} \sum_j (\cosh^2 \beta - \sinh^2 \beta \sigma_{j-1}^z \sigma_{j+1}^z) \sigma_j^x. \] (11)

3. Quantum to classical mapping
The converse mapping from a quantum Hamiltonian to classical dynamics can be formulated as follows [31, 32, 33]. Consider a quantum spin system that can be expressed in the basis of eigenstates of \( \{\sigma_j^z\}_j \) as \( H_{\sigma\sigma'} \). It is necessary to impose the conditions of negative semi-definiteness of off-diagonal elements
\[ H_{\sigma\sigma'} \leq 0 \ (\sigma \neq \sigma') \] (12)
and positive semi-definiteness of the eigenvalues,
\[ H\phi^{(0)} = 0, \] (13)
where $\phi^{(0)}$ is the ground-state eigenvector. The latter condition can always be satisfied by a shift of the energy standard. Under these conditions, the matrix $W$ defined by

$$W_{\sigma\sigma'} = -e^{-H_0(\sigma)/2} H_{\sigma\sigma'} e^{H_0(\sigma')/2}$$  \hspace{1cm} (14)

can be regarded as the transition matrix of a classical stochastic process of the Ising model $H_0(\sigma)$ whose elements are defined by

$$H_0(\sigma) = -2 \log \phi^{(0)}_\sigma.$$  \hspace{1cm} (15)

This last definition is valid because the ground-state eigenvector $\phi^{(0)}$ has all its elements positive

$$\phi^{(0)}_\sigma > 0$$  \hspace{1cm} (16)

due to the Perron-Frobenius theorem that applies to matrices with the properties described in equation (12). Notice that the prescription (15) has been inspired by the relation

$$\phi^{(0)}_\sigma = e^{-\beta H_0(\sigma)/2}$$  \hspace{1cm} (17)

in the classical-to-quantum mapping. It is also interesting that the present quantum-to-classical mapping does not change the spatial dimension in contrast to the Suzuki-Trotter decomposition or the path-integral formulation of quantum mechanics, by which the effective spatial dimension increases by one.

The classical Ising Hamiltonian $H_0(\sigma)$ defined by equation (15) has in general many-body long-range interactions with $2^N$ coefficients

$$H_0(\sigma) = \text{const} - \sum h_j \sigma_j - \sum J_{ij} \sigma_i \sigma_j - \cdots - J_N \sigma_1 \sigma_2 \cdots \sigma_N.$$  \hspace{1cm} (18)

The reason is that equation (15) must be satisfied by all possible values of $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$, and there are $2^N$ of them. Hence $H_0(\sigma)$ should have $2^N$ coefficients in front of various products of spin variables as they appear in equation (18). We set up $2^N$ linear equations for these coefficients, the solution of which gives, in general, non-vanishing values for all coefficients. This is in sharp contrast to the classical-to-quantum mapping, in which short-range interactions are mapped to short-range interactions. Since the many-body long-range interactions in equation (18) are hard to simulate, we may conclude that classical simulation of the quantum system is not efficient.

4. Conclusion

We have reformulated the mapping between classical stochastic dynamics of the Ising model and a quantum system in stationary state. It has been shown that classical stochastic dynamics with fixed temperature can be efficiently simulated by a quantum system whereas quantum systems cannot necessarily be efficiently simulated by classical dynamics as long as the present quantum-to-classical mapping is concerned. The present results indicate that simulated annealing, if the temperature is changed slowly, may be efficiently simulated by quantum annealing if a control parameter in the quantum system, typically the transverse field, is changed slowly or adiabatically. The reverse process to simulate quantum annealing with a slow change of a control parameter by simulated annealing with a slow decrease of temperature is not necessarily efficient. It may be premature to conclude only from this result that quantum annealing is superior to simulated annealing because other formulations of classical-quantum correspondence may be possible in which the present conclusion does not hold. It is nevertheless important to have established that the present method yields asymmetric correspondence between classical stochastic dynamics and quantum mechanics.
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