Re‘class’ification of ‘quant’ified classical simulated annealing

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Abstract. We discuss a classical reinterpretation of quantum-mechanics-based analysis of classical Markov chains with detailed balance, that is based on the quantum-classical correspondence. The classical reinterpretation is then used to demonstrate that it successfully reproduces a sufficient condition for cooling schedule in classical simulated annealing, which has the inverse-logarithm scaling.

1. Introduction
Theoretical properties of simulated annealing [1] have been extensively studied in the 1980s [2, 3]. One of the main issues in those research activities was regarding the annealing schedule: How should one decrease temperature $T(t)$ as a function of time $t$ in order to finally arrive at a globally optimum solution? Geman and Geman [4] were the first to obtain an answer, which states a sufficient condition of the form $T(t) \geq O(1/\log t)$. The inverse-logarithm scaling turned out to be universal, in the sense that it is also sufficient for many variants of simulated annealing and some other algorithms. Hajek [5] proved a necessary and sufficient condition which also has the inverse-logarithm form, showing that one cannot do the cooling any faster than that while guaranteeing global optimality.

Somma et al., in their recent contribution [6], have shown that the inverse-logarithm scaling of simulated annealing can also be obtained via the adiabatic condition [7] of a related quantum-mechanical system. The relationship between the original Markov chain in simulated annealing and the quantum system is established via the so-called classical-quantum mapping or quantum-classical correspondence [8, 9, 10]. In this paper, we discuss a classical reformulation of quantum equivalent of a classical Markov chain with detailed balance, in order to elucidate mathematical structure of the correspondence between a Markov chain and its quantum equivalent, without making reference to quantum mechanics. We also discuss another classical reformulation of the argument deriving the optimal inverse-logarithm scaling of annealing schedule [6] (see also [11]), which is based on the quantum adiabatic theorem.

This paper is organized as follows. In section 2 we first provide a basic formulation of classical Markov chains with detailed balance, and derive its $\alpha$-representation. A local linear approximation of the time evolution in terms of $\alpha$-representation is also discussed. Our derivation of the inverse-logarithm scaling of simulated annealing is discussed in section 3. A “chasing” view of simulated annealing, that is based on the local linear approximation based on the $0$-representation, and a bound of the largest negative eigenvalue are used in the derivation.
In section 4 we discuss relation between our formulation and the stochastic matrix form decomposition, which is defined and discussed extensively in [9]. Section 5 concludes the paper.

2. Basic formulations

2.1. Markov chains

Let $S$ denote a state space, which is a finite set of cardinality $N$. Let $E$ be an “energy function” defined on $S$, which associates a state $i \in S$ with its energy $E_i$. Then, one can define a probability distribution on $S$, in terms of a probability vector $\bar{\rho} = (\bar{\rho}_i)$, as

$$\bar{\rho}_i = \frac{e^{-\beta E_i}}{Z}, \quad Z = \sum_{i \in S} e^{-\beta E_i},$$

which is the Gibbs-Boltzmann distribution induced by the energy function $E$, with $\beta > 0$ a parameter corresponding to the inverse temperature.

Let us consider an undirected graph $G$ with $S$ its vertex set and an edge set $L$. We assume $G$ to be a connected graph, without self-edge (loop). We define a transition matrix $M = (m_{ij})$ as

$$m_{ij} = \begin{cases} w_{ij} e^{(E_j - E_i)/2} & (ij) \in L \\ -\sum_{k: (ik) \in L} m_{ki} & (i = j) \\ 0 & \text{(otherwise)} \end{cases},$$

where $W = (w_{ij})$ is a symmetric matrix with $w_{ij} > 0$ for $(ij) \in L$. On the basis of the transition matrix $M$, one can define a continuous-time Markov chain, as

$$\dot{\rho} = M \rho.$$

The connectedness of the graph $G$ induces irreducibility of the Markov chain. The Markov chain is also aperiodic, so that it is ergodic, and therefore bears a unique equilibrium distribution. The Gibbs-Boltzmann distribution (1) is the equilibrium distribution of the Markov chain, since $M \bar{\rho} = 0$ holds.

The formulation presented here is general, including various typical systems as special cases. For example, conventional Ising spin systems are described by letting $S = \{-1, 1\}^n$ with $N = 2^n$ and $L$ having an $n$-dimensional hypercubic structure. Metropolis and Glauber dynamics are implemented by letting

$$w_{ij} \propto \max \left\{ e^{E_j-E_i}/2, \ e^{E_i-E_j}/2 \right\},$$

and

$$w_{ij} \propto \frac{1}{e^{E_j-E_i}/2 + e^{E_i-E_j}/2},$$

respectively, as mentioned in [9].

2.2. $\alpha$-representation

We discuss a different representation of the continuous-time Markov chain (3), in view of the classical-to-quantum mapping utilized in [6]. Although the quantum reformulation mapped from a classical Markov chain makes use of square roots of probabilities $\{\sqrt{\rho_i}\}$, we here discuss a slightly more generalized expression which is based on the so-called $\alpha$-representation of $\rho$.

Definition. We define the $\alpha$-representation $\psi^{(\alpha)} = (\psi^{(\alpha)}_i)$ of $\rho$ as

$$\psi^{(\alpha)}_i = \frac{2}{1 - \alpha} \rho_i^{(1-\alpha)/2}.$$
The concept of \( \alpha \)-representation is originally introduced in information geometry [12, 13], in order to discuss intrinsic geometrical structures of statistical manifolds. Taking square roots of probabilities corresponds to considering 0-representation. Although not used in this paper, 1-representation is defined as

\[
\psi_i^{(1)} = \log \rho_i. \tag{7}
\]

We next derive an expression of the Markov chain in terms of the \( \alpha \)-representation. One has

\[
\dot{\psi}_i^{(\alpha)} = \rho_i^{-(1+\alpha)/2} \sum_{j \in S} m_{ij} \rho_j^{(1+\alpha)/2} \psi_j^{(\alpha)}, \tag{8}
\]

which is rewritten, in a vector-matrix form, as

\[
\dot{\psi}^{(\alpha)} = \frac{1 - \alpha}{2} H^{(-\alpha)} \psi^{(\alpha)}, \tag{9}
\]

where the matrix \( H^{(\alpha)} \) is defined as

\[
H^{(\alpha)} = (\Psi^{(\alpha)})^{-1} M \Psi^{(\alpha)}, \tag{10}
\]

with \( \Psi^{(\alpha)} = \text{diag}(\psi_i^{(\alpha)}) \). Clearly, eigenvalues of the matrix \( H^{(\alpha)} \) are the same as those of \( M \). The elements of the matrix \( H^{(-\alpha)} = (h_{ij}^{(-\alpha)}) \) are given by

\[
h_{ij}^{(-\alpha)} = \begin{cases} 
  w_{ij} e^{\beta (E_j - E_i)/2} \left( \frac{1}{\psi_i^{(\alpha)}} \right)^{-1} \psi_j^{(-\alpha)} & (ij \in L) \\
  - \sum_{k: (ik) \in L} w_{ki} e^{\beta (E_i - E_k)/2} & (i = j) \\
  0 & (\text{otherwise})
\end{cases} \tag{11}
\]

and consequently,

\[
\tilde{h}_{ij}^{(-\alpha)} = h_{ij}^{(-\alpha)} |_{\rho = \tilde{\rho}} = \begin{cases} 
  w_{ij} e^{\alpha (E_j - E_i)/2} & (ij \in L) \\
  - \sum_{k: (ik) \in L} w_{ki} e^{\beta (E_i - E_k)/2} & (i = j) \\
  0 & (\text{otherwise})
\end{cases}. \tag{12}
\]

The above expression evidently shows that the 0-representation is special in our formulation, in that the matrix \( H^{(-\alpha)} = H^{(-\alpha)} |_{\rho = \tilde{\rho}} \) becomes symmetric when \( \alpha = 0 \), that is, under the 0-representation. The fact that the 0-representation symmetrizes the transition matrix \( M \) was also mentioned in [14], in order to state that eigenvalues of \( M \) are all real. It should be noted that the matrix \( H^{(-\alpha)} \) is dependent on \( \psi^{(\alpha)} \) via \( \Psi^{(-\alpha)} \) and therefore \( H^{(0)} \) does not symmetric at \( \rho \neq \tilde{\rho} \) in general.

2.3. Time evolution

We discuss linearization of the \( \alpha \)-representation of the dynamical equation. Starting from the nonlinear dynamics

\[
\dot{\psi}_i^{(\alpha)} = \frac{1 - \alpha}{2} \left( \frac{1}{\psi_i^{(\alpha)}} \right)^{-1} \left( \frac{1}{\psi_j^{(\alpha)}} \right)^{2/(1-\alpha)} \sum_{j \in S} m_{ij} \left( \psi_j^{(\alpha)} \right)^{2/(1-\alpha)}, \tag{13}
\]
and considering a small perturbation $\delta \psi^{(\alpha)}$ around $\psi^{(\alpha)}$, we obtain the following linearized system which describes time evolution of $\delta \psi^{(\alpha)}$:

$$
\dot{\delta \psi_i^{(\alpha)}} = \left( \psi_i^{(\alpha)} \right)^{(1+\alpha)/(1-\alpha)} \sum_{j \in S} m_{ij} \left( \psi_j^{(\alpha)} \right)^{(1+\alpha)/(1-\alpha)} \delta \psi_j^{(\alpha)} - \frac{1 + \alpha}{2} \left[ \left( \frac{\psi_i^{(\alpha)}}{2} \right)^{2/(1-\alpha)} \sum_{j \in S} m_{ij} \left( \psi_j^{(\alpha)} \right)^{(2/(1-\alpha)} \right] \delta \psi_i^{(\alpha)} + o \left( \| \delta \psi^{(\alpha)} \| \right).
$$

(14)

In particular, observing that the second term of the right-hand side of (14) vanishes at the Gibbs-Boltzmann distribution $\bar{\rho}$, irrespective of the value of $\alpha$, the linearization around the equilibrium point becomes, ignoring higher-order terms,

$$
\delta \dot{\psi_i^{(\alpha)}} = \bar{H}(-\alpha) \delta \psi_i^{(\alpha)}.
$$

(15)

Equation (15) states that the matrix $\bar{H}(-\alpha)$ governs the local dynamics described in terms of $\alpha$-representation in the vicinity of the equilibrium distribution $\bar{\rho}$. It should be noted that the right-hand side of (14) is in general not a projection of $H(-\alpha) \delta \psi^{(\alpha)}$ onto the manifold of probability distributions in $\alpha$-representation, defined as

$$
\sum_{i \in S} \left( \frac{1 - \alpha}{2} \psi_i^{(\alpha)} \right)^{2/(1-\alpha)} = 1.
$$

(16)

3. Simulated annealing

3.1. Relaxation in annealing

With the inverse temperature $\beta$ fixed, the distribution following the Markov chain relaxes toward the Gibbs-Boltzmann distribution. The basic idea behind simulated annealing is that by gradually reducing the temperature one can arrive at a distribution which concentrates on a set of minimum-energy states. Thus, by performing simulations of the Markov chain with a proper cooling schedule, one expects to obtain minimum-energy states with probability close to 1. One of the basic questions regarding simulated annealing is to determine the cooling schedule which guarantees convergence to minimum-energy states.

We wish to study this problem via the linearized local dynamics in $\alpha$-representation (15), with $\alpha = 0$. Intuitively, our expectation is that if simulated annealing works well the distribution should stay very close to instantaneous equilibrium distributions as $\beta$ is changed slowly enough. If it is the case, then arguments that are based on the local linear approximation around the equilibrium (15) will be justified. Since the coefficient matrix $\bar{H}(0)$ is symmetric, all eigenvalues are real, so that the local dynamics around equilibrium is a simple linear relaxation toward the equilibrium, with negative eigenvalues of $\bar{H}(0)$ governing the speed of relaxation. In simulated annealing the instantaneous equilibrium distribution is also slowly drifting as $\beta$ changes. One can therefore expect to obtain a minimum-energy distribution only if the drift is slow enough so that the relaxation process is managed to catch up with the drift. What is important for successful convergence of simulated annealing is thus the largest negative eigenvalue of $\bar{H}(0)$.

3.2. Bound on largest negative eigenvalue

We let

$$
\mathcal{M} = (bI + \chi \bar{H}(0))^N,
$$

(17)

where $\chi = e^{-\beta d/2}/w_{\text{max}}$, with $d = \max_{i,j} |E_i - E_j|$ and $w_{\text{max}} = \max_{(ij) \in L} w_{ij}$, is to make diagonal elements of $\chi \bar{H}(0)$ nondiverging as $\beta$ gets large, and where

$$
b = 1 + \max_{i \in S} \sum_{k:(ki) \in L} \frac{w_{ki}}{w_{\text{max}}}
$$

(18)
is chosen so that \( bI + \chi \bar{H}(0) \) becomes a non-negative matrix. Irreducibility of the original Markov chain guarantees \( \mathcal{M} \) to be a (strictly) positive matrix.

The following theorem for positive matrices, due to Hopf [15] in its operator form, is applied to obtain an upper bound of the largest negative eigenvalue.

**Theorem 1** Let \( A = (a_{ij}) \) be a square matrix that is positive, i.e., \( a_{ij} > 0 \) holds for all \( i, j \). Then the maximum eigenvalue \( \lambda_0 \) of \( A \) and any other eigenvalues \( \lambda \) satisfy the inequality

\[
|\lambda| \leq \frac{\kappa - 1}{\kappa + 1} \lambda_0, \tag{19}
\]

where

\[
\kappa = \max_{i,j,k} \frac{a_{ik}}{a_{jk}}. \tag{20}
\]

All positive elements of the matrix \( bI + \chi \bar{H}(0) \) are bounded from below by \( \min\{1, w_{\min} \chi\} \), where \( w_{\min} = \min_{(ij) \in L} w_{ij} \), and \( w_{\min} \chi \) actually gives the lower bound for not too small values of \( \beta \). A lower bound of the minimum element of \( \mathcal{M} \) is thus \( (w_{\min} \chi)^N \). Alternatively, the matrix \( bI + \chi \bar{H}(0) \) is upper bounded componentwise by the matrix \( (b - 1)I + 11^T \), where \( 11^T \) is an all-1 matrix, so that an upper bound of the maximum element of \( \mathcal{M} \) is given by \( (3N)^N \). An upper bound of the parameter \( \kappa \) is therefore evaluated as

\[
\kappa \leq \left( \frac{3N}{w_{\min} \chi} \right)^N. \tag{21}
\]

Note that symmetry of the matrix \( bI + \chi \bar{H}(0) \), and hence of \( \mathcal{M} \), makes the argument of bounding \( \kappa \) straightforward, thereby demonstrating efficiency of the 0-representation.

Let \( \lambda \) be a negative eigenvalue of \( \bar{H}(0) \). Since we know that \( \bar{H}(0) \) has a zero eigenvalue which is the largest, applying theorem 1 yields

\[
(b + \chi \lambda)^N \leq \frac{\kappa - 1}{\kappa + 1} b^N, \tag{22}
\]

and consequently,

\[
\lambda \leq -\frac{2b}{N(\kappa + 1)} \leq -\frac{2b(w_{\min} \chi)^N}{N[(3N)^N + (w_{\min} \chi)^N]} \leq -\frac{b(w_{\min} \chi)^N}{N(3N)^N}, \tag{23}
\]

where we used the inequality \( 1 - [(\kappa - 1)/(\kappa + 1)]^{1/N} \geq 2/[N(\kappa + 1)] \) for \( \kappa, N \geq 1 \). To make clear its dependence on \( \beta \), we rewrite it as

\[
\lambda \leq -\delta e^{-\beta N(d + d')} / 2, \quad \delta = \frac{b}{N(3N)^N}, \tag{24}
\]

where we have taken into account possible dependence of \( w_{ij} \) on \( \beta \), by assuming that

\[
\frac{w_{\min}}{w_{\max}} \geq e^{-\beta d' / 2}, \quad d' \geq 0 \tag{25}
\]

holds.
3.3. Simulated annealing as a chase of target

From now on we assume the inverse temperature $\beta$ to be a function of time $t$, and consider speed of drift of the instantaneous equilibrium distribution $\bar{\psi}(0)$. We have

$$\left\| \dot{\bar{\psi}}^{(0)} \right\|^2 = \text{Cov}(E) \dot{\beta}^2 \leq C^2 e^{-\beta g/2} \dot{\beta}^2,$$

where $g$ is an energy gap between the lowest and the second lowest energies in $\{E_i; \ i \in S\}$, and where $C > 0$ is a constant independent of $\beta$.

Now the problem is recast into the problem of “chasing” a drifting target (see figure 1), whose velocity is no more than $C e^{-\beta g/2} \dot{\beta}$. The speed of the chaser is no less than $|\lambda|r$, where $r$ is the “distance” between the chaser and the target, because the speed is determined by gradient-descent of a potential surface induced by $\bar{H}^{(0)}$. In view of the adiabatic theorem, which lays the basis of the quantum-mechanics-based analysis of simulated annealing [6], we assume that $r$ is small throughout the process, so that the local linear approximation of the dynamics is valid.

We wish to obtain a sufficient condition for $\beta$, as a function of time $t$, such that $r$ tends to 0 as $t \to \infty$ and $\beta \to \infty$. With a modest amount of foresight, we assume that $r$ approaches zero as $r \sim r_0 t^{-\gamma}$ with $0 < \gamma < 1$. Since the speed of the chaser should be larger than that of the target, as a sufficient condition one has

$$\delta r_0 e^{-\beta N(d+d')/2} t^{-\gamma} > C e^{-\beta g/2} \dot{\beta}.$$  

(27)

Solving it for $\beta$, we obtain for large enough $t$,

$$\beta < \frac{2(1 - \gamma)}{N(d + d') - g} \log t + O(1).$$  

(28)

For consistency, the difference of the speeds of the chaser and the target is equal to $\dot{r}$, which should scale as $t^{-\gamma-1}$, yielding $\gamma = g/[N(d + d')]$. Collecting these results and ignoring non-dominant terms, one finally obtains

$$\beta^{-1} = T(t) > \frac{N(d + d')}{2 \log t}$$  

(29)

as a sufficient condition for simulated annealing to converge to a minimum-energy distribution.
4. Stochastic matrix form decomposition

The stochastic matrix form (SMF) decomposition, defined in [9], is a key to establishing the classical-to-quantum mapping. In this section, we briefly discuss relation between our formulation and the SMF decomposition.

The SMF decomposition of $H^{(\alpha)}$ is given by

$$H^{(\alpha)} = \sum_{(ij) \in L} w_{ij} H^{(\alpha)}_{ij},$$

(30)

with

$$H^{(\alpha)}_{ij} = e^{\beta(E_i - E_j)/2} \left[ \left( \psi^{(\alpha)}_i \right)^{-1} \psi^{(\alpha)}_j \mathcal{E}_{ij} - \mathcal{E}_{jj} \right] + e^{\beta(E_i - E_j)/2} \left[ \left( \psi^{(\alpha)}_j \right)^{-1} \psi^{(\alpha)}_i \mathcal{E}_{ji} - \mathcal{E}_{ii} \right],$$

(31)

where $\mathcal{E}_{ij}$ is a matrix with $(i, j)$ element being 1 and others being 0. Let $\bar{H}^{(\alpha)}$ denote the matrix evaluated at the equilibrium distribution of the Markov chain, that is, $\bar{H}^{(\alpha)} = H^{(\alpha)}_{ij}|_{\rho = \bar{\rho}}$. When $\alpha = 0$, it becomes

$$\bar{H}^{(0)}_{ij} = \mathcal{E}_{ij} + e^{\beta(E_i - E_j)/2} \mathcal{E}_{ii} - e^{\beta(E_j - E_i)/2} \mathcal{E}_{jj}. $$

(32)

The matrix $\bar{H}^{(0)}_{ij}$ is symmetric.

The $\alpha$-representation of the Gibbs-Boltzmann distribution, $\bar{\psi}^{(\alpha)}$, is an eigenvector of the matrix $\bar{H}^{(-\alpha)}_{ij}$ with eigenvalue 0, that is,

$$\bar{H}^{(-\alpha)}_{ij} \bar{\psi}^{(\alpha)} = 0$$

(33)

holds. This condition corresponds to the detailed-balance condition of the original formulation of the Markov chain. Note that it is consistent with the fact that $\bar{\psi}^{(\alpha)}$ is an eigenvector of the matrix $\bar{H}^{(-\alpha)}$ with eigenvalue 0.

5. Conclusion

In this paper, we have discussed a classical reinterpretation of the quantum-mechanics-based analysis of classical simulated annealing [6], that is based on the quantum-classical correspondence [8, 9, 10]. We have provided a reformulation of a Markov chain with detailed balance via the $\alpha$-representation, as well as its local linear approximation of time evolution. It has been shown that the local linear approximation preserving the eigenvalues of the original Markov chain (equation (15)) is valid only in the vicinity of the equilibrium distribution. On the basis of the 0-representation-based reformulation, we have shown that the inverse-logarithm scaling of temperature in simulated annealing that guarantee optimality is successfully reproduced on the basis of our formulation, without recourse to quantum adiabatic theorem.

We believe that usefulness of the $\alpha$-representation of Markov chains with detailed balance goes well beyond just deriving the inverse-logarithm scaling, and hope that our reformulation helps shed light on the usefulness of the $\alpha$-representation in more general context.

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