BALANCE OF RECURRENCE ORDERING TIME-INHOMOGENEOUS MARKOV CHAINS WITH APPLICATION TO SIMULATED ANNEALING*

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Abstract

We define a notion of *order of recurrence* for the states and transitions of a general class of time-inhomogeneous Markov chains with transition probabilities proportional to powers of a small vanishing parameter. These orders are shown to satisfy a *balance equation* across every *edge cut* in the associated graph. The resulting *order balance equations* allow computation of the orders of recurrence of the states, and thereby the determination of the asymptotic behavior of the Markov chain.

The method *of optimization by simulated annealing* is a special case of such Markov processes, and can therefore be treated by means of these balance equations. In particular, in this special situation we show that there holds a *detailed balance* of order of recurrence across *every edge* in the graph. Moreover, the sum of the order of recurrence of a state and its cost is shown to be a constant in each connected set of recurrent states. By this approach, we determine the necessary and sufficient condition on the "rate of cooling" to guarantee that a minimum of the optimization problem is hit with *probability one.* Moreover, the rates of convergence of the probabilities can be deduced from the orders of recurrence.

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1 INTRODUCTION

We consider the class of time-inhomogeneous Markov chains whose transition probabilities can be represented as *powers* of a time-varying parameter $\epsilon(t)$.

Let X be a finite state space and consider a time-inhomogeneous Markov chain $x(t)$ whose transition probabilities $p_{ij}(t) := P(x(t+1) = j | x(t) = i)$, are given by,

$$p_{ij}(t) \quad = \quad c_{ij}\epsilon(t)^{V_{ij}}, \quad \forall i, j \in X, \quad i \neq j \text{ and } t \in Z^{+} \tag{1}$$

where,

$$V_{ij} \geq 0, \quad \forall i, j \in X, \quad i \neq j, \tag{2}$$

$$c_{ij} \geq 0, \quad \forall i, j \in X, \quad i \neq j, \text{ and } \sum_{j \neq i} c_{ij} = 1 \forall i, \tag{3}$$

$$0 < \epsilon(t) \leq 1, \quad \forall t \in Z^{+}, \tag{4}$$

and

$$p_{ii}(t) \quad := \quad 1 - \sum_{\substack{j \in X \\ j \neq i}} p_{ij}(t).$$

Given an initial probability distribution $\pi_i(0) := P(x(0) = i)$, let

$$\pi_i(t) \quad := \quad P(x(t) = i)$$

be the probability distribution of $x(t)$, and

$$\pi_{ij}(t) \quad := \quad P(x(t) = i, x(t+1) = j)$$

be the probability of a *transition* from state i to state j at time t.

Our interest centers on determining the asymptotic properties of $\{\pi_i(t), i \in X\}$ and the process $\{x(t)\}$. To this end we define the *order of recurrence of state* $i \in X$, denoted β_i, as follows:

$$\begin{aligned}
\beta_i \quad &:= \quad -\infty \qquad \text{if } \sum_t \pi_i(t) + \infty, \\
&:= \quad p^{-} \qquad \text{if } p = \sup\left\{c \geq 0 : \sum_t \epsilon(t)^c \pi_i(t) = +\infty\right\} \text{ and } \sum_t \epsilon(t)^p \pi_i(t) + \infty, \\
&:= \quad p \text{ if } p = \max\left\{c \geq 0 : \sum_t \epsilon(t)^c \pi_i(t) = +\infty\right\},
\end{aligned}$$

(i.e., if the supremum is achieved.

If $\beta_i = -\infty$, we shall say that state i is *transient*, otherwise we shall say that it is *recurrent*.

In a similar way, we define the *order of recurrence of the transition from i to j*, β_{ij}, by,

$$\begin{aligned}
\beta_{ij} &:= -\infty \text{ if } \sum_t \pi_{ij}(t) + \infty, \\
&:= p^- \text{ if } p = \sup\{c \geq 0 : \sum_t \epsilon(t)^c \pi_{ij}(t) = +\infty\} \text{ and} \\
&\qquad \sum_t \epsilon(t)^p \pi_{ij}(t) + \infty, \\
&:= p \text{ if } p = \max\{c \geq 0 : \sum_t \epsilon(t)^c \pi_{ij}(t) = +\infty\} \\
&\qquad \text{i.e., if the supremum is achieved.}
\end{aligned}$$

Again we say that the *transition from i to j is transient if $\beta_{ij} = -\infty$, and recurrent* otherwise.

In the sequel, we distinguish between p^- and p. For convenience, we shall use the following straightforward conventions:

(i) p is regarded as *strictly* larger than p^- which in turn is regarded as *strictly* larger than $p - \delta$ for $\delta > 0$, i.e., $p > p^- > p - \delta$, for $\delta > 0$. (Hence, for example, $\max(p, p^-) = p$.)

(ii) $p^- - c := (p - c)^-$, and $p^- + c := (p + c)^-$.

As we show in this paper, the β_i's and β_{ij}'s are quite adequate to provide considerable information about the asymptotic behavior of the process $x(t)$, and furthermore, their properties can be deduced quite simply and elegantly. They therefore serve as a convenient "sufficient statistic" regarding the sequences $\{\pi_i(t), t \in Z^+\}$ and $\{\pi_{ij}(t), t \in Z^+\}$.

We show in Theorem 2.2 that the β_{ij}'s satisfy a *balance equation across every edge cut* in the graph associated with the Markov chain. The resulting *order balance equations* then yield the asymptotic properties of the Markov chain.

Then we turn to the method of *optimization by simulated annealing* which has been the subject of much recent interest, see [1-8]. We prove in Theorem 3.2 that in this special situation there actually holds a *detailed balance* across every *edge*, i.e., $\beta_{ij} = \beta_{ji}$. We show in Theorem 3.3 that this implies that the order of recurrence decreases as the cost of a state increases; the sum of the order and cost being a constant in each connected set of recurrent states. We obtain in Theorem 4.6 the necessary and sufficient condition on the rate of cooling in order for the algorithm to hit the minimum of the optimization problem *with probability one*. This extends the result of Hajek [5] who has previously shown the convergence of the algorithm *in probability*.

Historical Background

Markov chains with transition probabilities proportional to powers of a time-*invariant* parameter have been addressed in the singular perturbations literature; see Delebecque [12]. The case where the small parameter is time-varying, and converging to zero asymptotically, has been studied earlier by Tsitsiklis [6]. He obtains tight bounds on $\{\pi_i(t)\}$ by using techniques different from those used here. The problem of optimization by simulated annealing, which gives rise to a special time-inhomogeneous Markov chain of the type described above, was introduced as a procedure for combinatorial optimization problems by Kirkpatrick, Gelatt, and Vecchi [1]. Subsequently, in a pioneering work, Geman and Geman [2] showed that simulated annealing would indeed converge in probability to a minimum of the optimization problem provided $\sum \epsilon(t)^\rho = +\infty$ for large enough ρ. Bounds on the value of ρ needed for convergence, as well as some finite time analysis, were provided by Mitra, Romeo, and Sangiovanni-Vincentelli [3], and Gidas [4]. The precise value of ρ which is both necessary and sufficient for convergence to the minimum was first determined by Hajek [5]. Gelfand and Mitter [8] have also studied the finite time behavior as well as the rate of convergence of the simulated annealing algorithm. Finally, Hajek [7] has studied the complexity of the annealing algorithm for some combinatorial optimization problems.

2 BALANCE EQUATIONS FOR THE ORDERS OF RECURRENCE

We shall say that j *is a neighbor of* i if $c_{ij} > 0$ in $(1,3)$, i.e., there is a *positive* probability of transition from i to j. Let N_i be the set of neighbors of i.

The following Lemma relates β_{ij} to β_i.

Lemma 2.1. *Relationship between β_{ij} and β_i*

$$\begin{aligned} (i)\beta_{ij} &= -\infty \text{ if } j \notin N_i, & (5a)\\ (ii)\beta_{ij} &= -\infty \text{ if } j \in N_i \text{ but } \beta_i < V_{ij} & (5b)\\ &= \beta_i - V_{ij} \text{ if } j \in N_i \text{ and } \beta_i \geq V_{ij}. \end{aligned}$$

Proof: Part (i) is immediate. Part (ii) follows from the Chapman-Kolmogorov equation,

$$\begin{aligned} \pi_{ij}(t) &= \pi_i(t)p_{ij}(t)\\ &= c_{ij}\epsilon(t)^{V_{ij}}\pi_i(t). \end{aligned}$$

The following Theorem describes a fundamental property of the orders of recurrence. It shows that there has to be a balance of the order of recurrence across every edge cut in the digraph associated with the Markov chain.

We make the following "almost monotonicity" assumption regarding the sequence $\{\epsilon(t)\}$.

Assumption (A1). *There exists a constant $M > 0$ such that $\epsilon(s) \leq M\epsilon(t)$ for all $s \geq t$.*

Theorem 2.2. *(Order balance across edge cuts.) Under Assumption A1,*

$$\max_{\substack{i\in A\\ j\in A^c}} \beta_{ij} = \max_{\substack{j\in A^c\\ i\in A}} \beta_{ji} \qquad \text{for every } A \subseteq X. \tag{6}$$

Proof: Let $\{\tau(n)\}_{n\geq 1}$ be the sequence of random times at which the Markov process moves from A to A^c, i.e., $x(\tau(n)) \in A$ and $x(\tau(n)+1) \in A^c$. Similarly, let $\{\sigma(n)\}_{n\geq 1}$ be the sequence of random times at which the Markov process moves from A^c to A. Then

$$\tau(n) < \sigma(n) < \tau(n+1), \tag{7}$$

where we have assumed, without loss of generality, that the Markov process starts in A, i.e., $x(0) \in A$ (and so $\tau(1) < \sigma(1)$).

Let $c \geq 0$ be arbitrary. Then due to Assumption A1,

$$\epsilon(\sigma(n))^c \leq M^c\epsilon(\tau(n))^c.$$

Let $I(\cdot)$ denote the indicator function. By taking expectations and using the Monotone Convergence Theorem, we get

$$\begin{aligned}
\sum_{t\geq 0}\epsilon(t)^c \sum_{\substack{j\in A^c\\ i\in A}} \pi_{ji}(t) &= \sum_{t\geq 0}\epsilon(t)^c EI(x(t)\in A^c, x(t+1)\in A),\\
&= E\sum_{t\geq 0}\epsilon(t)^c I(x(t)\in A^c, x(t+1)\in A),\\
&= E\sum_{n\geq 1}\epsilon(\sigma(n))^c\\
&\leq M^c E\sum_{n\geq 1}\epsilon(\tau(n))^c,\\
&= M^c E\sum_{t\geq 0}\epsilon(t)^c I(x(t)\in A, x(t+1)\in A^c),\\
&= M^c \sum_{t\geq 0}\epsilon(t)^c EI(x(t)\in A, x(t+1)\in A^c),\\
&= M^c \sum_{t\geq 0}\epsilon(t)^c \sum_{\substack{i\in A\\ j\in A^c}} \pi_{ij}(t).
\end{aligned}$$

On the other hand, using the second inequality in Eq. (7), we have

$$M^c\epsilon(\sigma(n))^c \;\geq\; \epsilon(\tau(n+1))^c,$$

which yields,

$$\begin{aligned}
E\sum_{n\geq 1}\epsilon(\sigma(n))^c &\geq M^{-c}E\sum_{n\geq 1}\epsilon(\tau(n+1))^c\\
&= M^{-c}E\sum_{n\geq 2}\epsilon(\tau(n))^c\\
&= M^{-c}\left[E\sum_{n\geq 1}\epsilon(\tau(n))^c - E\epsilon(\tau(1))^c\right],\\
&\geq M^{-c}\left[E\sum_{n\geq 1}\epsilon(\tau(n))^c - \max_{t\geq 0}\epsilon(t)^c\right]\\
&\geq M^{-c}E\sum_{n\geq 1}\epsilon(\tau(n))^c - \epsilon(0)^c \qquad \text{(using } M\epsilon(0)\geq\epsilon(t)).
\end{aligned}$$

Combining the inequalities above, we get

$$M^c\sum_{\substack{i\in A\\ j\in A^c}}\sum_{t\geq 0}\epsilon(t)^c\pi_{ij}(t) \geq \sum_{\substack{j\in A^c\\ i\in A}}\sum_{t\geq 0}\epsilon(t)^c\pi_{ji}(t) \;\geq\; M^{-c}\sum_{\substack{i\in A\\ j\in A^c}}\sum_{t\geq 0}\epsilon(t)^c\pi_{ij}(t) - \epsilon(0)^c. \quad (8)$$

If the left-hand side is finite when $c = 0$, then so is the center term: whereas if the center term is finite when $c = 0$, then so is the right-hand side. This shows that

$$\max_{\substack{i\in A\\ j\in A^c}} \beta_{ij} = -\infty \quad \Leftrightarrow \quad \max_{\substack{j\in A^c\\ i\in A}} \beta_{ji} = -\infty.$$

Consider next the case $\max_{\substack{i\in A\\ j\in A^c}} \beta_{ij} = p^- > 0$. Then, for every $\delta > 0$ the right side of Eq. (8) is $+\infty$ when c is replaced by $p - \delta$. Since $\delta > 0$ is arbitrary, it follows that

$$\max_{\substack{j\in A^c\\ i\in A}} \beta_{ji} \quad \geq \quad p^- = \max_{\substack{i\in A\\ j\in A^c}} \beta_{ij}.$$

On the other hand, if $\max_{\substack{i\in A\\ j\in A^c}} \beta_{ij} = p \geq 0$, then with the choice of $c = p$, the right-hand side of Eq. (8) is $+\infty$, and therefore so is the center term. This shows that

$$\max_{\substack{j\in A^c\\ i\in A}} \beta_{ji} \quad \geq \quad p = \max_{\substack{i\in A\\ j\in A^c}} \beta_{ij}.$$

In any case therefore,

$$\max_{\substack{j\in A^c\\ i\in A}} \beta_{ji} \quad \geq \quad \max_{\substack{i\in A\\ j\in A^c}} \beta_{ij}.$$

A similar argument applied to the first inequality in Eq. (8) shows the reverse inequality, completing the proof. (The case $\max_{\substack{i\in A\\ j\in A^c}} \beta_{ij} = +\infty$ can also be treated. It needs only a slight modification.)

The following example illustrates how the resulting solution of the orders of recurrence generally yields the asymptotic properties of the Markov chain.

Example 2.3 See Figure 1. Let

$$\begin{aligned}
X &= \{5, 3, 2, 1\}, \\
V_{ij} &= j - i \text{ if } j \geq i, \\
&= 0 \qquad \text{if } j \leq i, \\
c_{13} &= c_{32} = c_{25} = 1, \\
c_{52} &= c_{51} = \tfrac{1}{2}, \\
c_{ij} &= 0 \text{ for all other } i, j, \\
\epsilon(t) &= 1/t^{1/3}.
\end{aligned} \tag{9}$$

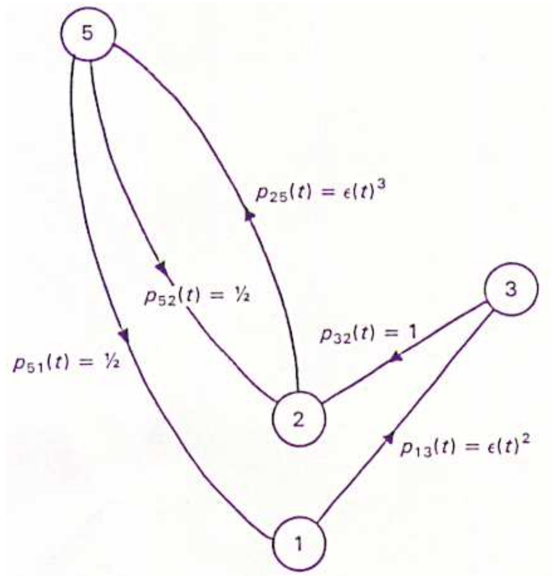

Figure 1: Markov chain of Examples 2.3 and 3.7.

It should be noted that if $\{\beta_i\}$ is a solution of the order balance equations, then $\{\beta_i + c\}$ is also a solution for every constant c, i.e., the solution set is translation invariant. To fix the particular solution, one needs to utilize the additional information provided by Eq. (9), $\epsilon(t) = 1/t^{1/3}$, as follows. Note that,

$$+\infty \quad = \quad \sum_{t\geq 1} \epsilon(t)^3 = \sum_i \left[\sum_{t\geq 1} \pi_i(t)\epsilon(t)^3 \right], \text{ which implies that } \max_i \beta_i \geq 3.$$

However,

$$+\infty \sum_{t\geq 1} \epsilon(t)^{3+\delta} \text{ for all } \delta > 0 \text{ which implies that } \beta_i < 3+\delta \text{ for all } \delta > 0, \text{ i.e., } \max_i \beta_i \leq 3.$$

Hence

$$\max_i \beta_i \quad = \quad 3,$$

which fixes the particular solution. Now by using the nodal order balance equations, i.e., the equations (6) derived from the choice of $A = \{i\}$ for

$i = 1, 2, 3, 5$, one can obtain the orders of recurrence,

$$\beta_1 = 2, \qquad \beta_2 = 3, \qquad \beta_3 = 0, \qquad \beta_5 = 0$$
$$\beta_{13} = \beta_{31} = \beta_{32} = \beta_{25} = \beta_{52} = \beta_{51} = 0.$$

From this, the asymptotic properties of the Markov chain, and, in particular, the fact that the Markov process converges in the sense of *Cesaro mean* to the state 2, can be easily deduced as follows. To see this, note that since $\beta_i < 2 + \delta$ for $i = 1, 3, 5$, then

$$\sum_t \epsilon(t)^{2+\delta} P(x(t) \neq 2) \quad = \quad \sum_t \epsilon(t)^{2+\delta} [\pi_1(t) + \pi_3(t) + \pi_5(t)] < \infty.$$

By Kronecker's Lemma (see Chung [9]), it follows that

$$\lim_N \epsilon(N)^{2+\delta} \sum_{t=1}^{N} P(x(t) \neq 2) = 0, \qquad (\text{ for } \delta < 1).$$

Noting that $\epsilon(N) = 1/N^{1/3}$, this leads to

$$\lim_N \frac{1}{N} \sum_{t=1}^{N} P(x(t) \neq 2) \quad = \quad 0.$$

Finally, using

$$\frac{1}{N} \sum_{t=1}^{N} P(x(t) = 2) + \frac{1}{N} \sum_{t=1}^{N} P(x(t) \neq 2) \quad = \quad 1,$$

it follows that,

$$\lim_N \frac{1}{N} \sum_{t=1}^{N} P(x(t) = 2) \quad = \quad 1.$$

The next example shows that in general it is *insufficient* to only consider cutsets derived from *singleton* sets A, as was done in Example 2.3.

Example 2.4. See Figure 2. Let

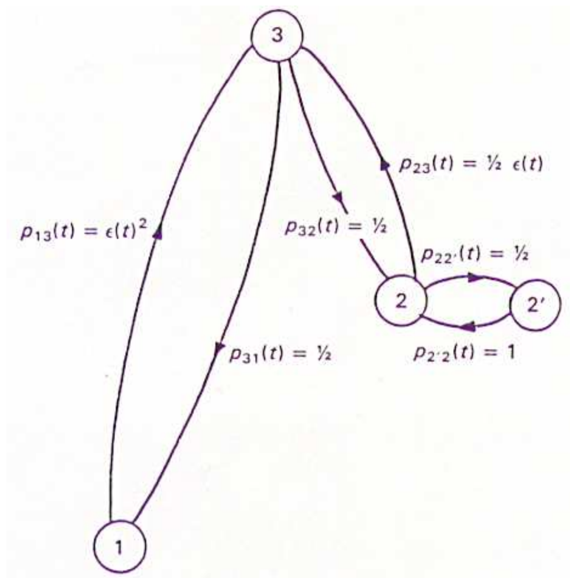

Figure 2: Markov chain of Examples 2.4.

$$
\begin{aligned}
X &= \{3, 2, 2', 1\}, \\
V_{13} &= 2, \\
V_{31} &= V_{32} = V_{22'} = V_{2'2} = 0, \\
V_{23} &= 1, \\
c_{13} &= c_{2'2} = 1, \\
c_{31} &= c_{32} = c_{23} = c_{22'} = \tfrac{1}{2}, \\
c_{ij} &= 0 \text{ for all other} i, j, \\
\epsilon(t) &= 1/t^{1/3}.
\end{aligned}
\tag{10}
$$

If we restrict attention to cutsets derived from setting $A = \{i\}$, for $i = 1, 2, 2', 3$, in the order balance equations (6), we get

$$
\begin{aligned}
\beta_{13} = \beta_{31} & \qquad \text{with cutset} A = \{1\}, \\
\max(\beta_{31}, \beta_{32}) = \max(\beta_{13}, \beta_{23}) & \qquad \text{with cutset} A = \{3\}, \\
\max(\beta_{23}, \beta_{22'}) = \max(\beta_{32}, \beta_{2'2}) & \qquad \text{with cutset} A = \{2\}, \\
\beta_{2'2} = \beta_{22'} & \qquad \text{with cutset } A = \{2'\}.
\end{aligned}
$$

As in the previous example, we can deduce from Eq. (10) that

$$\max_i \beta_i = 3.$$

It is then easy to check that the assignments,

$$\begin{aligned}\beta_1 &= 3,\\ \beta_3 &= \beta_2 = \beta_{2'} = 1,\\ \beta_{13} &= \beta_{31} = 1,\\ \beta_{23} &= 0,\\ \beta_{32} &= \beta_{22'} = \beta_{2'2} = 1,\end{aligned}$$

satisfy all the above equations, as well as the relationships between β_i and β_{ij} shown in Lemma 2.1.

However, they do *not* satisfy the balance equation,

$$\beta_{32} = \beta_{23} \qquad \text{with cutset} A = \{1, 3\},$$

and are therefore not the right assignments. By including the additional condition $\beta_{32} = \beta_{23}$, the correct solution is obtained as

$$\beta_1 = 3, \beta_3 = 1, \beta_2 = \beta_{2'} = 2,$$
$$\beta_{13} = \beta_{31} = \beta_{23} = \beta_{32} = 1, \beta_{22'} = \beta_{2'2} = 2,$$

(see also Theorems 3.2 and 3.3).

This shows that to realize the full power of the order balance equations one generally needs to utilize *all* edge cuts.

Remark 2.5 It is easy to check that the preceding order balance Theorem 2.2, and in fact all the results in this paper, continue to remain valid if Eq. (1) is replaced by

$$p_{ij}(t) = c_{ij} g_{ij}(t) \epsilon(t)^{V_{ij}} \qquad \text{for } i \neq j$$

where

$$0 < \gamma \;\; \leq \;\; g_{ij}(t) \leq \gamma^{-1}.$$

The introduction of $g_{ij}(t)$ does not affect any of the results, since it really does not change *orders* of recurrence.

3 DETAILED ORDER BALANCE IN SIMULATED ANNEALING

In the remainder of this paper, we apply the order balance equations (6) to the method of *optimization by simulated annealing.* We show that there actually holds a *detailed order balance across every edge.* This gives necessary and sufficient conditions for the optimization algorithm to hit the global minimum with probability one.

First we describe the method of optimization by simulated annealing.

Let X be a finite set and suppose that there is a cost function $W : X \to R$. To each state $i \in X$, associate a *nonempty neighborhood* $N_i \subseteq X$ with $i \notin N_i$. Suppose that at time t, the current state is $x(t) = i$. Choose a neighbor $j \in N_i$, with probability c_{ij}. If $W_j \leq W_i$ then set $x(t+1) = j$. Otherwise, if $W_j > W_i$, set $x(t+1) = j$ with probability $\epsilon(t)^{W_j - W_i}$, and $x(t+1) = i$ with probability $(1 - \epsilon(t)^{W_j - W_i})$.

This yields a time-inhomogeneous Markov chain with

$$\begin{aligned} p_{ij}(t) &= c_{ij}\epsilon(t)^{[W_j - W_i]^+} \qquad \text{for } j \neq i, \\ p_{ii}(t) &= 1 - \sum_{j \neq i} p_{ij}(t), \end{aligned}$$

where $x^+ := \max(0, x)$. The sequence $\{\epsilon(t)\}$ is called the *cooling schedule*; see Hajek [5].

Thus, we have a Markov chain of the type satisfying Eqs. (1-4), with the special choice of V_{ij} as

$$V_{ij} \;:=\; [W_j - W_i]^+. \tag{11}$$

In what follows, we will assume that "neighborhoods are symmetric."

Assumption A2.

$$j \in N_i \quad \Leftrightarrow \quad i \in N_j.$$

Lemma 3.1. *Let i and j be neighbors with $W_j \geq W_i$. Then*

$$(i) \qquad \beta_{ji} = \beta_j \tag{12a}$$

$$\begin{aligned} (ii) \qquad \beta_{ij} &= \beta_i + W_i - W_j, \qquad \textit{if } (\beta_i + W_i - W_j) \geq 0, \\ &= -\infty, \qquad \textit{if } (\beta_i + W_i - W_j) < 0. \end{aligned} \tag{12b}$$

$$(iii) \qquad \beta_j \leq \beta_i \tag{12c}$$

$$\begin{aligned} (iv) \qquad & \beta_{ij} \leq \beta_{ji}. \textit{ Further, if } \beta_j \geq 0, \textit{ then} \\ & \beta_i + W_i \leq \beta_j + W_j. \end{aligned} \tag{12d}$$

Proof: Since $W_j \geq W_i$, we have from Eq. (11),

$$\begin{aligned} V_{ji} &= [W_i - W_j]^+ = 0, \\ V_{ij} &= [W_j - W_i]^+ = W_j - W_i. \end{aligned}$$

Then (i) and (ii) follow by appropriate substitution in Eq. 5b. To prove (iii), note from Lemma 2.1 that $\max_k \beta_{ik} \leq \beta_i$. Then applying the order balance Theorem 2.2 with the choice of A equal to the *singleton set* $\{i]$ gives $\beta_i \geq \max_{k\neq i} \beta_{ik} = \max_{k\neq i} \beta_{ki} \geq \beta_{ji} = \beta_j$. To prove (iv) apply the order balance Theorem 2.2 with the choice of $A = \{j\}$. Noting $\beta_j \geq \beta_{jk}$ for all k, we get

$$\beta_{ji} = \beta_j \geq \max_{k\neq j} \beta_{jk} = \max_{k\neq j} \beta_{kj} \geq \beta_{ij}.$$

Substituting appropriately for β_{ij} and β_{ji} from (i), (ii), and (iii), we get (iv).

It is convenient in the sequel to associate a *graph* with the Markov process, and to use the notation of graph theory; see Bondy and Murthy [10]. Let G be the graph with vertex set X and having an edge between vertices i and j if and only if $j \in N_i$.

Our first result for simulated annealing is that order balance holds across *every edge* in the graph. This is much stronger than order balance across every *edge cut*. We shall refer to this property as *detailed order balance* in analogy with the usage of such an expression for reversible Markov chains which occur in queueing networks; see Kelly [11].

Theorem 3.2. *Detailed order balance for simulated annealing. Under Assumption A1 and A2,*

$$\beta_{ij} = \beta_{ji} \qquad \text{for every } i, j \in X. \tag{13}$$

Proof: Let R be the set of recurrent states (i.e., those i with $\beta_i \geq 0$) and T be the set of transient states (i.e., those i with $\beta_i = -\infty$).

Clearly the theorem is true for $i, j \in T$ because $\beta_i = \beta_j = -\infty$, and by Lemma 2.1 it follows that $\beta_{ij} = \beta_{ji} = -\infty$.

Next consider states $i \in R$ and $j \in T$. Since $j \in T$, by Lemma 2.1 we have $\beta_{jk} = -\infty$ for all k. Applying the order balance Theorem 2.2 with the choice of A as the *singleton set* $\{j\}$ gives,

$$-\infty = \max_{k\neq j} \beta_{jk} = \max_{k\neq j} \beta_{kj} \geq \beta_{ij},$$

showing that $\beta_{ij} = \beta_{ji} = -\infty$. Thus, we are only left to consider $i, j \in R$.

Note that if $j \notin N_i$, then from the "symmetric neighborhood" Assumption A2, it follows that $i \notin N_j$. Lemma 2.1 then shows that $\beta_{ji} = \beta_{ij} = -\infty$ in such a case. Therefore, we need only consider $i, j \in R$ with $j \in N_i$.

Let $G[R]$ be the subgraph of G induced by the vertex set R, i.e., the graph whose vertex set is R and whose edge set is the set of edges of G with both ends in R.

We can assume without loss of generality that i and j belong to a *common connected component* of $G[R]$ (otherwise i and j would not be neighbors). So fix attention on a *particular connected component* $G[C]$ of $G[R]$. We will show in Theorem 3.3 which follows that there is a constant $\alpha(C)$ (i.e., depending possibly on the choice of the connected component C) such that,

$$\beta_i + W_i = \alpha(C), \qquad \text{for all} i \in C. \tag{14}$$

Suppose for the time being that Eq. (14) has been established; it then follows immediately that for $i, j \in C$,

$$\beta_i + W_i \quad = \quad \beta_j + W_j.$$

Assume without loss of generality that $W_j \geq W_i$. Then Eq. (11) and Lemma 3.1 give the series of implications:

$$\begin{aligned} \beta_{ji} = -\infty \quad &= \quad \beta_j = -\infty = \beta_j + W_j = -\infty = \beta_i + W_i = -\infty \\ &= \quad \beta_i + W_i - W_j < 0 = \beta_{ij} = -\infty = \beta_{ji} = \beta_{ij} = -\infty \end{aligned}$$

and,

$$\begin{aligned} \beta_{ji} \geq 0 = \beta_j = \beta_{ji} \geq 0 \quad &= \quad \beta_i + W_i - W_j = \beta_j \geq 0 = \beta_{ij} = \beta_i + W_i - W_j \\ &= \quad \beta_{ij} = \beta_j = \beta_{ij} = \beta_{ji}. \end{aligned}$$

Therefore, the equality of β_{ji} and β_{ij} will follow if Eq. (14) holds.

Thus, to conclude the proof of this theorem, we need only show that Eq. (14) holds.

Thus to conclude the proof of this theorem, we need only show that Eq. (14) is valid for every connected component $G[C]$ of $G[R]$. This is the content of the following Theorem 3.3.

Theorem 3.3. *β is a potential on C. Assume A1 and A2. For every connected component $G[C]$ of $G[R]$, the subgraph of G induced by the set R of recurrent states, there exists a constant $\alpha(C)$ such that*

$$\beta_i + W_i = \alpha(C), \qquad \textit{for all } i \in C. \tag{15}$$

Proof: It will be convenient to use the following (picturesque) notation. We will say that

(i) *j is an uphill (respectively downhill) neighbor of i* if $j \in N_i$ and $W_j \geq W_i$ (respectively $W_j \leq W_i$).

(ii) *$(i_0, i_1, \ldots, i_p)$ is an uphill (respectively downhill) path* if it is a path, i.e., $i_{k+1} \in N_{i_k}$ and $i_k \neq i_j$ for $k \neq j$, and each i_{k+1} is an uphill (respectively downhill) neighbor of i_k.

(iii) *j is uphill (respectively downhill) of i* if there is an uphill (respectively downhill) path from i to j. We will denote by D_i the set of states downhill of i.

(iv) *i is a local minimizer of W* if $W_j = W_i$ for every $j \in D_i$.

Definition 3.4.

(i) A non-empty set S is said to be a valley if whenever $(i_0, i_1, \ldots, i_p)$ is a downhill path with $i_0 \in S$, then $i_k \in S$ for $1 \leq k \leq p$. We will then say that S satisfies property (V).

(ii) β is said to be a potential on the set S if there exists a constant $\alpha(S)$ such that $\beta_i + W_i = \alpha(S)$ for all $i \in S$. We will then say that S satisfies property (P).

Consider a particular connected component $G[C]$. Let $\Gamma := \{A \subseteq C : A = D_i$ for some local minimizer $i\}$ be the sets of local minimizers, and let us list its elements as $\Gamma = \{A_1, A_2, \ldots, A_m\}$. Note that since elements are not repeated, $A_l \cap A_p = \phi$ for $l \neq p$.

Consider a particular set A_l and let Σ_l be the collection of nonempty subsets of C which contain A_l and which satisfy (V,P). We will show that Σ_l is *non-empty* by showing that $A_l \in \Sigma_l$. Clearly A_l satisfies property (V), since the set of local minimizers contains all states downhill of its members. Thus, we need to show that A_l satisfies property (P). Let $A_l = D_k$ for some local minimizer k. Hence $W_j = W_k$ for all $j \in A_l$. In particular, for all $i, j \in A_l$, we have $W_i = W_j$. Hence, to show property (P) we only need to show that $\beta_i = \beta_j$ for all $i, j \in A_l$. If i and j are neighbors, this follows from Eq. (12c). This equality then extends to all of A_l since it is connected. Thus, $A_l \in \Sigma_l$, proving that Σ_l is nonempty.

Let "$\subseteq$" denote the set containment relation, and let $(\Sigma_l, \subseteq)$ be the resulting partial order of elements of Σ_l. Every chain in $(\Sigma_l, \subseteq)$ has an upper bound which is formed by taking the union; so there exists a *maximal* element of $(\Sigma_l, \subseteq)$, called H_l. Thus, there is no set satisfying (V,P) which contains H_l as a *strict* subset.

Let $\Delta := \{A \subseteq C : A = H_l\}$ for some $l\}$ be a collection of maximal elements, one from each Σ_l. List its elements as $\Delta = \{S_1, S_2, \ldots, S_r\}$. Note that $S_l \cap S_p = \phi$ for $l \neq p$, since otherwise $S_k \cup S_p$ would satisfy (V,P), violating the maximality of S_l and S_p.

Thus we have a situation where,

(i)

$$\cup_{l=1}^{r} S_l \supseteq \{i : i \text{ is a local minimizer}\}, \tag{16}$$

(ii) each S_l satisfies (V,P),

(iii) each S_l is maximal, i.e., there is no $\overline{S} \subseteq_{\neq} S_l$ which also satisfies (V,P).

Let $\alpha(S_l)$ be the constant such that,

$$\beta_i + W_i = \alpha(S_l) \qquad \text{for all} i \in S_l.$$

Note that if $\alpha(S_l) = \alpha(S_p)$ for $p \neq l$, then $S_l \cup S_p$ would also satisfy (V,P), which in turn would violate the maximality of S_l and S_p. Thus,

$$\alpha(S_l) \neq \alpha(S_p), \qquad \text{for } l \neq p.$$

So let us assume without loss of generality that

$$\alpha(S_1)\alpha(S_2) < \ldots < \alpha(S_r). \tag{17}$$

We will now show that actually $S_1 = C$, i.e., Δ is a singleton set and its only element is C.

The proof is by contradiction. Suppose not; i.e., $S_1 \neq C_1$. Then $S_1^c \cap C \neq \phi$ and we claim that there has to exist some j, a neighbor of S_1, which extends property (P); i.e., there exists $j \in N_i \cap S_1^c \cap C$ for some $i \in S_1$ such that

$$\beta_j + W_j \quad = \quad \alpha(S_1). \tag{18}$$

The proof of this also is by contradiction. Suppose not; i.e., there does not exist such a j. Then,

$$\beta_j + W_j \neq \beta_i + W_i (= \alpha(S_1)) \qquad \text{for every } i \in S_1 \text{ and every } j \in N_i \cap S_1^c \cap C.$$

This also means

$$\beta_j \quad \neq \quad \beta_i + W_i - W_j.$$

Since S_1 satisfies (V), every neighbor $j \in S_1^c$ of $i \in S_1$ has to satisfy

$$W_j \quad > \quad W_i.$$

From Eq. (12a), it follows that

$$\beta_{ji} = \beta_j \neq \beta_i + W_i - W_j.$$

There are two cases. If the right-hand side above is nonnegative, then from Eq. (12b) it follows that it is equal to β_{ij}, and so $\beta_{ji} \neq \beta_{ij}$. On the other hand, if the right-hand side is strictly negative, then from Eq. (12b) it follows that $\beta_{ij} = -\infty$, which again is different from $\beta_{ji} = \beta_j \geq 0$. In any case, therefore.

$$\beta_{ji} \neq \beta_{ij}, \qquad \text{for all } i \in S_1 \text{ and } j \in N_i \cap S_1^c \cap C. \tag{19}$$

From Eq. (12d), however, we know that $\beta_{ij} \leq \beta_{ji}$ since $i \in D_j$. But since equality cannot hold due to Eq. (19), it follows that

$$\beta_{ij} < \beta_{ji}, \qquad \text{for all} i \in S_1 \text{ and } j \in N_i \cap S_1^c \cap C.$$

But then, noting that for $j \in N_i^c \cup C^c$ and $i \in N_i$, $\beta_{ij} = -\infty$ and also $\beta_{ji} = -\infty$, we have

$$\max_{\substack{i \in S_1 \\ j \in S_1^c}} \beta_{ij} = \max_{\substack{i \in S_1 \\ j \in S_1^c \cap N_i \cap C}} \beta_{ij} < \max_{\substack{i \in S_1 \\ j \in S_1^c \cap N_i \cap C}} \beta_{ji} = \max_{\substack{i \in S_1 \\ j \in S_1^c}} \beta_{ji},$$

which contradicts the order balance Theorem 2.2. Hence, our assumption (19) is false, and there exists a $j \in N_i \cap S_1^c \cap C$, for some $i \in S_1$, which satisfies Eq. (18).

Now we obtain the contradiction to $S_1^c \cap C \neq \phi$ by showing that Eq. (18) is impossible.

Consider a $j \in N_i \cap S_1^c \cap C$ for some $i \in S_1$ satisfying Eq. (18). Note that $j \notin S_l$ for $l > 1$, for otherwise, if $j \in S_l$ then $\alpha(S_l) = \beta_j + W_j = \alpha(S_1)$ contradicting Eq. (17). Since j does not belong to any S_l, $1 \leq l \leq r$, it cannot be a local minimizer due to Eq. (16). Hence, there exists at least one downhill path from j to some local minimizer. This local minimizer can either be in S_l for $l > 1$ or in S_1. Hence, there are two possibilities: either,

(i) there exists a downhill path $(j = i_0, i_1, \ldots, i_p)$ with $i_p \in S_l$ for $l > 1$, or

(ii) every downhill path $(j = i_0, i_1, \ldots, i_p)$ with i_p a local minimizer has $i_p \in S_1$.

If (i) is true, then by Eq. 12d), we have

$$\alpha(S_1) = \beta_j + W_j \geq \beta_{i_1} + W_{i_1} \geq \beta_{i_2} + W_{i_2} \geq \ldots \geq \beta_{i_p} + W_{i_p} = \alpha(S_l), \quad \text{for } l > 1$$

which contradicts Eq. (17). On the other hand, if (ii) is true, then $\overline{S} := S_1 \cup D_j$ satisfies (V). It also satisfies (P) since if $k \in D_j$, then there is a downhill path $(j = i_0, \ldots, i_m = k, i_{m+1}, \ldots, i_p)$ with $i_p \in S_1$. But then $\beta_k + W_k = \alpha(S_1)$, since by Eq. (12d),

$$\alpha(S_1) = \beta_j + W_j \geq \beta_k + W_k \geq \beta_{i_p} + W_{i_p} = \alpha(S_1).$$

However $\overline{S}$ then contradicts the maximality of S_1. Thus, our assumption that $S_1^c \cap C \neq \phi$ is false, and $S_1 = C$. But then C satisfies (P), proving the theorem.

The detailed order balance and the potential nature of the β_i's allow one to fill in the values of the β_i's, as the following Corollary 3.5 shows.

Corollary 3.5. *Computing β's along uphill and downhill paths. Fix a state $i \in X$.*

(i) If there exists an uphill path from i to j, then

$$\beta_j = \beta_i + W_i - W_j, \qquad \text{if } \beta_i + W_i - W_j \geq 0, \tag{20a}$$
$$= -\infty, \qquad \text{if } \beta_i + W_i - W_j < 0. \tag{20b}$$

(ii) If $\beta_i \geq 0$ and there exists a downhill path from i to j, then

$$\beta_j = \beta_i + W_i - W_j. \tag{20c}$$

(iii) If $\beta_i \geq 0$ and there exists a path $(i = i_0, i_1, \ldots, i_p = j)$ with $\max_{1 \leq l \leq p}(W_{i_l} - W_i) \leq \beta_i$, then

$$\beta_j = \beta_i + W_i - W_j. \tag{20d}$$

Proof: We will first prove the corollary when i and j are neighbors. For Eq. (20a), we see from Eq. (12d) that $\beta_j \geq \beta_i + W_i - W_j \geq 0$, and so i and j are in the same connected component. Theorem 3.3 then gives Eq. (20a).

For Eq. (20b), from Eqs. (12a,12b), we have $-\infty = \beta_{ij} = \beta_{ji} = \beta_j$.

For Eq. (20c), note that i and j belong to the same connected component, and so the result follows from Theorem 3.3.

The result Eq. (20d) follows from (i) and (ii) when i and j are neighbors.

The extension to the general case where i and j are not neighbors is obtained in a straightforward manner by considering an uphill path (or downhill path, or path satisfying the conditions for (iii)), $(i = i_0, i_1, \ldots, i_p = j)$ and applying the above results for (i) or (ii) to each pair (i_{k-1}, i_k) of neighbors.

Given an initial *known* value of β at some vertex, the procedure of Corollary 3.5 can be applied repeatedly to fan out and fill in other values of the β's. If β_i has been determined, we can determine the β values of all *uphill* neighbors of i, and also the β values of all *downhill* neighbors *but only if* $\beta_j \geq 0$. Thus, the algorithm stops when it *cannot* find any *new* state which cannot be reached *except* by going downhill from an already determined transient state.

The algorithm therefore determines all values of β in the *connected component* C in which the initial vertex lies, and also determines all transient states which are uphill of C. To determine the orders of recurrence of *all states*, one thus needs to know the order of recurrence of *one* state in *each* connected component.

The following example illustrates the necessity of knowing the value of the order of recurrence of *at least* one state in each connected component.

Example 3.6. See Figure 3. Let

$$\begin{aligned} X &= 1, 2, 3, \\ W_i &= i, \\ c_{13} &= c_{23} = 1, \\ c_{31} &= c_{32} = \frac{1}{2}, \\ c_{ij} &= 0 \qquad \text{for all other } i, j, \\ \epsilon(t) &= 1/(t+1). \end{aligned}$$

Then the complete set of order balance equation (6) obtained by utilizing

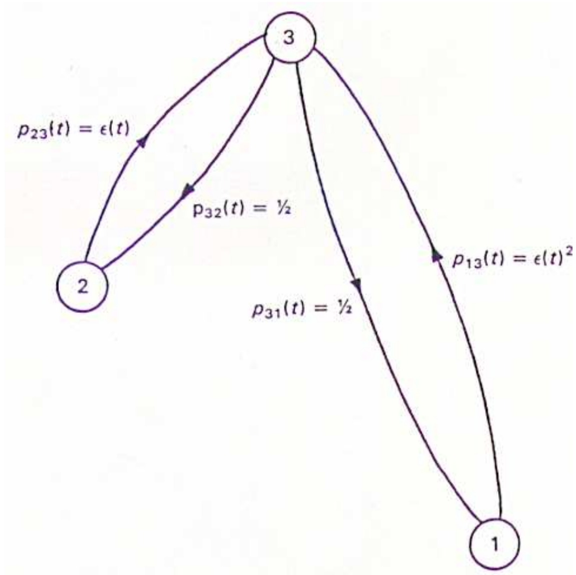

Figure 3: Markov chain of Examples 3.6.

all cutsets is

$$\begin{aligned} \beta_{23} &= \beta_{32}, \\ \beta_{31} &= \beta_{13}, \\ \max(\beta_{23}, \beta_{13}) &= \max(\beta_{32}, \beta_{31}). \end{aligned}$$

These balance equations are never adequate to determine the orders of recurrence. (They do not depend in any way on the particular choice of the sequence $\{\epsilon(t)\}$, and so several solutions are possible depending on the particular sequence employed. For example, at the least, these equations are invariant under translation by a sufficiently large scalar). So we usually proceed (see Examples 2.3, 2.4) by utilizing the additional knowledge that

$$\max_i \beta_i = 1 \qquad (\text{since } \epsilon(t) = 1/(t+1)). \tag{21}$$

However, this is generally not enough to determine all the orders of recurrence uniquely, since the assignments,

$$\beta_1 = 1, \qquad \beta_3 = -\infty, \qquad \beta_2 = \alpha,$$
$$\beta_{ij} = -\infty \qquad \text{for all} i, j,$$

satisfy all the above equations for *every* $\alpha \in \{-\infty\} cup [0, 1^-]$.

The difficulty here is that one does not know the order of recurrence of *even* one state in the connected component $\{2\}$. However,

$$\begin{aligned}
\pi_2(t) &\geq \pi_2(1)p_{22}(1)p_{22}(2)\cdots p_{22}(t-1) \\
&= \pi_2(1)(1-\epsilon(1))(1-\epsilon(2))\cdots(1-\epsilon(t-1)) \\
&= \pi_2(1)\left(1-\frac{1}{2}\right)\left(1-\frac{1}{3}\right)\cdots\left(1-\frac{1}{t}\right) \\
&= \frac{\pi_2(1)}{t}
\end{aligned}$$

shows that $\beta_2 \geq 0$, and therefore that $\beta_2 \in [0, 1^-])$.

The next example shows that when the *symmetric neighborhood* Assumption A2 is violated, *detailed balance* need not hold, and neither need $\beta_i + W_i = constant$ hold for all i in a connected component.

Example 3.7: See Figure 1. Let

$$\begin{aligned}
X &= \{5, 3, 2, 1\}, \\
W_i &= i, \\
c_{13} &= c_{32} = c_{25} = 1, \qquad c_{52} = c_{51} = \frac{1}{2}, \qquad c_{ij} = 0 \text{ otherwise}, \\
\epsilon(t) &= 1/t^{1/3}.
\end{aligned}$$

The neighborhoods are not symmetric; in particular, $3 \in N_1$ but $1 \notin N_3$. Using $V_{ij} = [W_j - W_i]^+$ shows that V_{ij} is the same as Example 2.3. Hence, as proved earlier,

$$\beta_1 = 2, \qquad \beta_2 = 3, \qquad \beta_3 = 0, \qquad \beta_5 = 0$$
$$\beta_{13} = \beta_{31} = \beta_{32} = \beta_{25} = \beta_{52} = \beta_{51} = 0$$

showing that

$$\beta_1 + W_1 = 3, \qquad \beta_2 + W_2 = 5, \qquad \beta_3 + W_3 = 3, \qquad \beta_5 + W_5 = 5.$$

It should be noted that the simulated annealing algorithm therefore converges in the sense of Cesaro mean to the state 2, which is *not* a minimizer of the cost.

4 NECESSARY AND SUFFICIENT CONDITIONS FOR SIMULATED ANNEALING TO HIT THE GLOBAL MINIMUM

Let

$$\begin{aligned} \underline{W} &:= \min_{i \in X} W_i = \text{ minimum of } W, \\ M &:= \{i \in X : W_i = \underline{W}\} = \text{ set of minimizers of } W. \end{aligned}$$

We will now determine necessary and sufficient conditions on the "cooling schedule" $\{\epsilon(t)\}$ in order that optimization by simulated annealing is guaranteed to hit a minimum of $\underline{W}$ with probability one, for all initial states, i.e.,

$$P(\text{there exists a } t \text{ with } x(t) \in M) = 1, \quad \text{for all initial states } x(0) \in X. \tag{22}$$

Note that this is *equivalent* to

$$\lim_{t \to \infty} [\min_{n \leq t} W(x(n))] = \underline{W} a.s., \qquad \text{for all initial states } x(0) \in X. \tag{23}$$

This objective Eq. (23) is reasonable if one is willing to *store* the least cost state already encountered by the algorithm in addition to present state.

The necessary and sufficient conditions that we obtain for Eqs. (22) and (23) are the same as those previously determined by Hajek [5] to be necessary and sufficient for the algorithm to converge *in probability* to the minimum.

The key step which takes us from knowledge of the orders of recurrence to the asymptotic behavior is the *Borel-Cantelli Lemma* (see Chung [9]), which says that,

$$\sum_t \pi_i(t) < +\infty = P(x(t) = i \text{ only finitely often}) = 1.$$

Definition 4.1. *(Order of a cooling schedule). Let*

$$\begin{aligned} \rho := p \qquad & \text{if } p = \max \left\{ c \geq 0 : \sum_t \epsilon(t)^c = +\infty \right\}, \\ := p^- \qquad & \text{if } p = \sup \left\{ c \geq 0 : \sum_t \epsilon(t)^c = +\infty \right\} \\ & \qquad \text{and } \sum_t \epsilon(t)^p + \infty. \end{aligned}$$

We shall call ρ the order of the cooling schedule.

Lemma 4.2.

$$\max_{i\in X} \beta_i \quad = \quad \rho.$$

Proof: For any $c \geq 0$,

$$\sum_t \epsilon(t)^c \quad = \quad \sum_{i\in X}\sum_t \pi_i(t)\epsilon(t)^c,$$

since $\sum_{i\in X}\pi_i(t) = 1$. Hence, if the left-hand side converges, then $\sum_t \pi_i(t)\epsilon(t)^c$ should converge for *all* $i \in X$, whereas if the left-hand side diverges, then $\sum_t \pi_i(t)\epsilon(t)^c$ should diverge for *at least one* $i \in X$, proving the Lemma.

Without loss of generality we will assume that the graph G is *connected.* (Otherwise we simply treat each connected component separately.)

Definition 4.3. *(Depth of an optimization problem). Let d^* be the smallest number with the property that for every $i \in X$ one can find a path ($i = i_0, i_1, \ldots, i_p$) ending in some minimizer $i_p \in M$ of W such that*

$$W_{i_k} - W_i \leq d^*, \qquad \text{for } k = 1, 2, \ldots, p. \tag{24}$$

We shall say that d^* is the depth of the optimization problem.

Assumption A3.

$$\lim_{t\to\infty} \epsilon(t) \quad = \quad 0.$$

Lemma 4.4. *(Sufficient condition for simulated annealing to hit a minimum). Assume A1, A2, and A3. If*

$$\sum_{t\geq 1} \epsilon(t)^{d^*} \quad = \quad +\infty,$$

then

(i) the condition (22), or equivalently (23), holds for all initial conditions $x(0) \in X$.

(ii) In fact,

$$\limsup_{N\to\infty} \frac{1}{N}\sum_{t=1}^{N} P(x(t) \in M) \quad = \quad 1.$$

Proof: Consider an arbitrary initial condition $x(0) \in X$. Note that,

$$\max_{i \in X} \beta_i \quad = \quad \rho \geq d^*.$$

We claim that

$$\beta_i = \rho \Rightarrow i \in M. \tag{25}$$

To prove this, consider an $i^* \in X$ at which β is a maximum, i.e., $\beta_{i^*} = \rho \geq d^*$. From the definition of d^*, there exists a path $(i = i_0, i_1, \ldots, i_p = j)$ with $j \in M$ such that $\max_{1 \leq k \leq p}(W_{i_k} - W_i) \leq d^*$. Corollary 3.5 shows that $\beta_j = \beta_i + W_i - W_j$. Noting that $\beta_j \leq \rho = \beta_i$, we have

$$\underline{W} \leq W_i \quad = \quad \beta_j - \beta_i + W_j \leq vW_j = \underline{W},$$

proving that $W_i = \underline{W}$ and thus the claim Eq. (25).

Now recall (from Theorem 3.2) our notation $G[R]$ for the subgraph of G induced by the set of recurrent states R. Hence, if $\{G(C_l) : 1 \leq l \leq m\}$ are the connected components of $G[R]$, then every path from C_l to C_p, with $l \neq p$, must pass through a vertex in T. However, since T is the set of transient states,

$$\sum_t P(x(t) \in T) \quad = \quad \sum_{i \in T} \sum_t \pi_i(t) < +\infty,$$

and so, by the Borel-Cantelli Lemma,

$$P(x(t) \in T \text{ for only finitely many } t) \quad = \quad 1. \tag{26}$$

This means that along almost every sample ω, the trajectory $\{x(t, \omega); t \geq 1\}$ can cross from one connected component of $G[R]$ to another only *finitely often*. Therefore, along almost every sample path, $\{x(t, \omega); t \geq 1\}$ *converges to some connected component*, i.e.,

$$x(t, \omega) \in C_{r(\omega)}, \qquad \text{for all} t \geq T(\omega), a.e. \omega,$$

where $r(\omega)$ is the (random) index of the connected component.

We will now show that,

$$C_l \cap M \quad = \quad \phi \Rightarrow \lim_t P(x(t) \in C_l) = 0. \tag{27}$$

To prove this, consider a connected component C_l, $1 \leq l \leq m$, for which $P(C_{r(\omega)} = C_l) > 0$. Then, $\lim_t P(x(t) \in C_l) =: \theta > 0$, which means that

$\sum_{i \in C_l} \pi_i(t) \geq \theta - \delta > 0$ for all $t \geq$ some τ. But then, $\sum_{i \in C_l} \sum_{t \geq \tau} \pi_i(t) \epsilon(t)^c \geq (\theta - \delta) \sum_{t \geq \tau} \epsilon(t)^c$, and by following the argument of Lemma 4.2, we can conclude that $\max_{i \in C_l} \beta_i = \rho$. Hence, from Eq. (25) it follows that $C_l \cap M \neq \phi$. Thus, we have shown that

$$P(C_{r(\omega)} = C_l) \quad > \quad 0 \Longrightarrow C_l \cap M \neq \phi,$$

which is equivalent to saying that

$$C_l \cap M = \phi \Longrightarrow P(C_{r(\omega)} = C_l) \quad = \quad 0.$$

The right-hand side above equation, however, implies the right-hand side of Eq. (27), thus proving Eq. (27).

Consider now a C_l containing a minimizer, i.e., a C_l such that

$$C_l \cap M \quad \neq \quad \phi.$$

Define,

$$D_l \quad := \quad C_l \cap M^c,$$

and let,

$$\gamma \quad := \quad \min_{i \in M^c} (W_i - \underline{W}),$$

be the difference between the least cost and the next to least cost. Consider some $i^* \in C_l \cap M$. Then $\beta_{i^*} \leq \rho$. For any other $i \in D_l$, it follows that

$$\beta_i \quad = \quad \beta_{i^*} + W_{i^*} - W_i \leq \beta_{i^*} - \gamma \leq \rho - \gamma.$$

Hence, if

$$\rho \quad = \quad p^{-} \text{ or} p,$$

then

$$\sum_t \pi_i(t) \epsilon(t)^{p - \gamma + \delta} < +\infty, \qquad \text{for all } \delta > 0, \text{ for all} i \in D_l.$$

Application of Kronecker's Lemma (see Chung [9]) using Assumption A3 gives

$$\lim_{N \to \infty} \epsilon(N)^{p - \gamma + \delta} \sum_{t=1}^{N} P(x(t) \in D_l) \quad = \quad 0,$$

i.e.,

$$\lim_{N\to\infty} (N\epsilon(N)^{p-\gamma+\delta}) \frac{1}{N} \sum_{t=1}^{N} P(x(t) \in D_l) \quad = \quad 0. \tag{28}$$

The next step is to show that

$$\lim_{N\to\infty} N\epsilon(N)^{p-\gamma+\delta} \quad > \quad 0. \tag{29}$$

Suppose Eq. (29) is not true. Then

$$\lim_{N\to\infty} N\epsilon(N)^{p-\gamma+\delta} \quad = \quad 0,$$

and so

$$\lim_{N\to\infty} \frac{1/N}{\epsilon(N)^{p-\gamma+\delta}} \quad = \quad +\infty,$$

i.e.,

$$\lim_{N\to\infty} \frac{(1/N)^{\frac{p-\delta}{p-\gamma+\delta}}}{\epsilon(N)^{p-\delta}}, = +\infty, \qquad \text{for all small} \delta > 0.$$

But since $\sum_{N\geq 1} \epsilon(N)^{p-\delta} = +\infty$ for small $\delta > 0$ (since $p - \delta < \rho$), this would imply that $\sum_{N=1}^{\infty} (1/N)^{\frac{p-\delta}{p-\gamma+\delta}} = +\infty$ for small $\delta > 0$, which is false.

Hence, Eq. (29) holds, and from Eq. (28)) we deduce that

$$\lim \infty_{N\to\infty} \frac{1}{N} \sum_{t=1}^{N} P(x(t) \in D_l) = 0, \text{ where} l \text{ is such that} C_l \cap M \neq \phi, \\ \text{and } D_l := C_l \cap M^c. \tag{30}$$

Now note that Eq. (26) implies that

$$\lim_t P(x(t) \in T) \quad = \quad 0. \tag{31}$$

Because of Eqs. (27), (30, and (31), it follows that

$$\liminf_N \frac{1}{N} \sum_{t=1}^{N} \pi_i(t) = 0, \qquad \text{for all } i \notin M.$$

But since

$$\frac{1}{N}\sum_{t=1}^{N} P(x(t) \in M) + \frac{1}{N}\sum_{t=1}^{N} P(x(t) \notin M) \quad = \quad 1,$$

it follows that

$$\limsup_{N\to\infty} \frac{1}{N}\sum_{t=1}^{N} P(x(t) \in M) \quad = \quad 1. \tag{32}$$

Clearly, this implies Eq. (22), for otherwise if $P(x(t) \in M^c \text{ for all } t \geq 1) =:$ $\mu > 0$, then we would also have

$$\limsup_{N\to\infty} \frac{1}{N}\sum_{t=1}^{N} P(x(t) \in M) \leq 1 - \mu < 1$$

which contradicts Eq. (32).

Hence, we have established the lemma.

Lemma 4.5. *(Necessary condition for simulated annealing to hit a minimum). Assume A1 and A2. If*

$$\sum_{t\geq 1} \epsilon(t)^{d^*} \quad < \quad +\infty,$$

then there exists an initial condition $x(0) \in X$ for which

$$P(x(t) \in M^c \text{ for every } t \geq 1) \quad > \quad 0. \tag{33}$$

Proof: Note first that ρd^*. Since d^* is the *smallest* number with the property given by Eq. (24), there exists a state i^* in X such that *whenever* $(i^* = i_0, i_1, \ldots, i_p)$ is a path with $i_p \in M$, then $\max_{1\leq k\leq p}(W_{i_k} - W_{i^*}) \geq d^*$. Consider such an i^*, and define,

$$\begin{aligned} Y \quad := \quad & \{i \in X : \text{ there exists a path } (i^* = i_0, i_1, \ldots, i_p = i) \\ & \text{with } \max_{1\leq k\leq p}(W_{i_k} - W_{i^*}) \leq \rho\}, \end{aligned}$$

and let

$$N(Y) \quad := \quad \{j \in X : j \in N_i \text{ for some } i \in Y\} \cap Y^c$$

be the set of neighbors of Y. Note that $N(Y)$ is nonempty. (Since Y^c contains M, and since G is connected there exists a neighbor of Y in Y^c).

We claim that

$$j \in N(Y) \quad = \quad W_j > W_{i^*} + \rho. \tag{34}$$

Otherwise, if $W_j \leq W_{i^*} + \rho$ for some $j \in N(Y)$, choose an $i \in Y$ such that $j \in N_i$. Now if $(i^* = i_0, i_1, \ldots, i_p = i)$ is a path with $\max_{1 \leq l \leq p}(W_{i_l} - W_{i^*}) \leq \rho$, then the extended path $(i^* = i_0, i_1, \ldots, i_p = i, i_{p+1} = j)$ is also a path with $\max_{1 \leq l \leq p+1}(W_{i_l} - W_{i^*}) \leq \rho$, contradicting the hypothesis that $j \notin Y$.

Now define

$$\begin{aligned} \tilde{p}_{ij}(t) &:= p_{ij}(t), \qquad \text{for } i \in Y \text{ and all } j, \\ &:= \frac{p_{ij}(t)}{\sum_{k \in Y} p_{ik}(t)}, \qquad \text{for } i \in N(Y), j \in Y, \end{aligned} \tag{35}$$

and consider the Markov process with initial condition $\tilde{x}(0) = i^*$, with state space

$$\tilde{X} \quad := \quad Y \cup N(Y), \tag{36}$$

and transition probabilities $\tilde{p}_{ij}(t)$. Note that

$$\tilde{X} \cap M \quad = \quad \phi. \tag{37}$$

We will call this new process $(\tilde{X}, \tilde{p})$ the *reflected process*, since it coincides with (X, p) in Y, and upon hitting $N(Y)$ is "reflected" back into Y with probabilities equal to the *conditional probabilities given that the* original process (X, p) has so moved back into Y upon leaving it.

Now $\tilde{p}_{ij}(t)$ can be written as,

$$\begin{aligned} \tilde{p}_{ij}(t) &= c_{ij} g_{ij}(t) \epsilon(t)^{V_{ij}}, \qquad \text{for } i \in Y \text{ and all} j, \text{ with } g_{ij}(t) := 1, \\ &= c_{ij} g_{ij}(t) \epsilon(t)^{V_{ij}}, \qquad \text{for } i \in N(Y), j \in Y, \text{ with} g_{ij}(t) := \frac{1}{\sum_{k \in Y} p_{ik}(t)}. \end{aligned}$$

Let $c := min\{c_{ij} : c_{ij} > 0\}$ and note that

$$p_{ik}(t) = c_{ik} \epsilon(t)^{V_{ik}} = c_{ik} \geq c > 0 \qquad \text{for } i \in N(Y), k \in Y \cap N_i,$$

since $W_i > W_k$ and so $V_{ik} = 0$. Hence,

$$1 \leq g_{ij}(t) \quad \leq \quad \frac{1}{c},$$

and so, by Remark 2.5, the results obtained so far also apply to the reflected process $(\tilde{X}, \tilde{p})$.

Denote the orders of recurrence of this reflected process by $\tilde{\beta}_i$.

We claim that,

$$\tilde{\beta}_j = -\infty, \qquad \text{for all} j \in N(Y). \tag{38}$$

To prove this, we first claim that,

$$\tilde{\beta}_i \leq \rho + W_{i^*} - W_i, \qquad \text{for all } i \in Y. \tag{39}$$

Suppose Eq. (39) is not true. Then for $i \in Y$, $\tilde{\beta}_i \rho + W_{i^*} - W_i$. Let $(i^* = i_0, i_1, \ldots, i_p = i)$ be a path with $\max_{1 \leq k \leq \rho}(W_{i_k} - W_{i^*}) \leq \rho$, which exists by assumption since $i \in Y$. But then the *reversed path*, $(i = i_p, i_{p-1}, \ldots, i_0 = i^*)$ is a path with $\max_{1 \leq k \leq \rho}(W_{i_k} - W_i) \leq \rho - W_i + W_{i^*}$. Hence, by Eq. (20d) it follows that $\tilde{\beta}_{i^*} = \tilde{\beta}_i + W_i - W_{i^*} > \rho$, which is impossible. This proves Eq. (39).

Now we can prove Eq. (38). Fix $j \in N(Y)$ and let $i \in Y \cap N_j$ be a neighbor. Then, by Eqs. (34) and (39),

$$\tilde{\beta}_i + W_i - W_j \leq \rho + W_{i^*} - W_j < 0.$$

This proves Eq. (38) because of Eq. (5b).

By definition Eq. (38) implies that

$$\sum_{t \geq 1} \tilde{\pi}_i(t) + \infty, \qquad \text{for all} i \in N(Y)$$

(where $\tilde{\pi}_i(t) := P(\tilde{x}(t) = i)$ are the probabilities corresponding to $(\tilde{X}, \tilde{p})$). Thus,

$$\sum_{t \geq 1} P(\tilde{x}(t) \in N(Y)) \quad < \quad +\infty.$$

By the Borel-Cantelli Lemma, it follows that

$$P(\tilde{x}(t) \in N(Y) \text{ only finitely often}) \quad = \quad 1.$$

Hence there exist some n and $\{(t_1, i_1), (t_1, i_2), \ldots, (t_n, i_n)\}$ with $i_l \in N(Y)$ for $1 \leq l \leq n$ such that

$$P(\tilde{x}(t_l) = i_l \text{ for } 1 \leq l \leq n \text{ and } \tilde{x}(t) \in Y \text{ for all } t \neq t_l) =: \tilde{\alpha} > 0.$$

Let

$$\theta(t) \quad := \quad \min_{\substack{i \in N(Y) \\ j \in Y}} p_{ij}(t) > 0.$$

Since $(\tilde{X}, \tilde{p})$ coincides with (X, p) in Y and on $N(Y)$ has transition probabilities equal to the probabilities conditioned on the reflection into Y, it follows that,

$$\begin{aligned} P(x(t_l) &= i_l \text{ for } 1 \leq l \leq n \text{ and } x(t) \in Y \text{ for all } t \neq t_l) \\ &\geq \theta(t_1)\theta(t_2)\cdots\theta(t_n)\tilde{\alpha} =: \alpha > 0. \end{aligned}$$

Hence,

$$P(x(t) \in Y \cup N(Y) \text{ for all } t \geq 1) \geq \alpha > 0.$$

Because of Eq. (36), it follows that

$$P(x(t) \in M \text{ for some } t \geq 1) \leq 1 - \alpha < 1.$$

The preceding two Lemmas 4.4 and 4.5 give the following necessary and sufficient condition for optimization by simulated annealing to hit a minimum with probability one.

Theorem 4.6. *(Necessary and sufficient condition for hitting a minimum). Assume A1, A2, A3. Then*

$$P(x(t)) \text{ hits a minimizer of } W \text{ for some } t) = 1, \qquad \text{for all } x(0) \in X, \tag{40}$$

if and only if,

$$\sum_{t \geq 1} \epsilon(t)^{d^*} \quad = \quad +\infty,$$

where d^* is the depth of the optimization problem.

Remark 4.7. *In fact the necessity of the condition (40) in Theorem 4.6 can be strengthened to say that*

$$\sum_{t \geq 1} \epsilon(t)^{d^*} < +\infty = \quad P(x(t)) \text{ never hits a minimizer of } W) > 0,$$
$$\text{for all } x(0) \in X$$

from which there is a path to a state such as i in the proof of Lemma 4.5 which does not pass through M. The proof of this fact is just based on noticing that since the graph of the Markov chain is connected, the state identified as i^* in Lemma 4.5 is hit with positive probability irrespective of the initial condition $x(0)$, and from i^* we have already seen in Lemma 4.5 that there is a positive probability of never reaching a minimizer.

Remark 4.8. *(Rate of convergence of probabilities). The orders of recurrence $\{\beta_i\}$ actually indicate the rate of convergence of the probabilities $\{\pi_i(t)\}$. For example, if*

$$\epsilon(t) := 1/t^{1/\rho}$$

and

$$\beta_i \quad = \quad p^- \text{ or } p,$$

then the conditions

$$\sum_t \frac{\pi_i(t)}{t^{(p+\delta)/\rho}} = \sum_{t \geq 1} \pi_i(t)\epsilon(t)^{p+\delta} < +\infty, \qquad \text{for all } \delta > 0$$

and

$$\sum_{t \geq 1} \frac{\pi_i(t)}{t^{(p-\delta)/\rho}} = \sum_{t \geq 1} \pi_i(t)\epsilon(t)^{p-\delta} = +\infty, \qquad \text{for all } \delta > 0 (\text{since } \rho \geq p^-)$$

indicate that $\frac{\pi_i(t)}{t^{p/\rho}}$ behaves (roughly) like $\frac{1}{t}$, i.e., $\pi_i(t)$ is roughly like $t^{(p/\rho)-1}$. This result is similar to those in Mitra, Romeo and Sangiovanni-Vincentelli [3].

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