QUASI–STATICALLY COOLED MARKOV CHAINS*†

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Abstract

We consider time–inhomogeneous Markov chains on a finite state–space, whose transition probabilities $p_{ij}(t) = c_{ij}\epsilon(t)^{V_{ij}}$ are proportional to powers of a vanishing small parameter $\epsilon(t)$. We determine the precise relationship between this chain, and the corresponding time–homogeneous chains $p_{ij} = c_{ij}\epsilon^{V_{ij}}$, as $\epsilon \searrow 0$. Let $\{\nu_i^\epsilon\}$ be the steady–state distribution of this time–homogeneous chain. We characterize the orders $\{\eta_i\}$ in $\nu_i^\epsilon = \Theta(\epsilon^{\eta_i})$. We show that if $\epsilon(t) \searrow 0$ slowly enough, then the time–wise occupation measures $\beta_i := \sup\{q > 0 \mid \sum_{t=1}^{\infty} \epsilon(t)^q \text{ Prob}(x(t) = i) = +\infty\}$, called the recurrence orders, satisfy $\beta_i - \beta_j = \eta_j - \eta_i$. Moreover, if $\mathcal{G} := \{\eta_i \mid \eta_i = \min_j \eta_j\}$ is the set of "ground states" of the time–homogeneous chain, then $x(t) \to \mathcal{G}$, in an appropriate sense, whenever $\eta(t)$ is "cooled" slowly. We also show that there exists a critical ρ^* such that $x(t) \to \mathcal{G}$ if and only if $\sum_{t=1}^{\infty} \epsilon(t)^{\rho^*} = +\infty$. We characterize this critical rate as $\rho^* = \max_{i \notin \mathcal{G}} \min_{i^* \in \mathcal{G}} \min_{p=(i=i_0,\ldots,i_N=i^*)} \max_{0 \le k \le N-1} (V_{i_k i_{k+1}} + \eta_{i_k} - \eta_i)$. Finally, we provide a graph algorithm for determining the orders $\{\eta_i\}$ and $\{\beta_i\}$, and the critical rate ρ^*.

1 Introduction

Consider a time–inhomogeneous Markov chain $\{x(t)\}$ with transition probabilities

$$p_{ij}(t) = c_{ij}\epsilon(t)^{V_{ij}}.$$

We are specifically interested in the case when the small parameter $\epsilon(t)$ converges to zero slowly. One expects the asymptotic behavior of this chain to be closely related to the behavior

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*Please address all correspondence to the third author.

†The research reported here has been supported in part by the U. S. Army Research Office under Contract No. DAAL–03–91–G–0182, and the Joint Services Electronics Program under Contract No. N00014–90–J1270.

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of the corresponding time–homogeneous chain,

$$p_{ij} = c_{ij}\epsilon^{V_{ij}}.$$

as $\epsilon \searrow 0$.

Indeed, this is the basis for the well known simulated annealing algorithm of Kirkpatrick *et al.* [1]. There, one has a cost function $\{W_i\}$ over the states, and the exponents V_{ij} are chosen as[1]

$$V_{ij} := [W_j - W_i]^+.$$

Suppose also that $c_{ij} > 0 \Leftrightarrow c_{ji} > 0$, i.e., the neighborhood structure is symmetric, and that the chain is irreducible. Then, the steady–state probabilities $\{\nu_i^\epsilon\}$, of the time–homogeneous chain, satisfy[2]

$$\nu_i^\epsilon = \Theta(\epsilon^{W_i - W^*}),$$

where

$$W^* = \min_j W_j.$$

As $\epsilon \searrow 0$, this steady–state distribution gets concentrated on the set of global minima,

$$\mathcal{G} := \{i \mid W_i = W^*\}.$$

In simulated annealing, the goal is to optimize the cost function W, i.e., to reach this global minimum set $\mathcal{G}$. In analogy with thermodynamics, the sequence $\{\epsilon(t)\}$ is called the "temperature schedule." One hopes that by running the time–inhomogeneous chain with the small parameter sequence $\epsilon(t)$ reduced to zero slowly, it will also converge to $\mathcal{G}$. One can then say that the chain has been "quasi–statically cooled." Results of this nature have been shown for simulated annealing in [2, 3, 4, 5, 6, 7].

In this paper we develop analogous results for the general time–inhomogeneous chain with arbitrary non–negative $\{V_{ij}\}$. We first characterize the "stationary orders" $\{\eta_i\}$, as in

$$\nu_i^\epsilon = \Theta(\epsilon^{\eta_i}) \qquad \text{as } \epsilon \searrow 0,$$

[1] $x^+ := \max(0, x)$.

[2] By this, we mean there exist constants $a_1 > 0$ and $a_2 > 0$ such that $a_1\epsilon^{W_i - W^*} \leq \nu_i^\epsilon \leq a_2\epsilon^{W_i - W^*}$ for all $\epsilon > 0$ sufficiently small.

of the steady–state distribution of the time–homogeneous chain.

Turn now to the time–inhomogeneous chain. Let

$$\pi_i(t) := \mathrm{Prob}(x(t) = i)$$

denote the occupation probability. Let us measure the time–wise occupation of a state i by[3]

$$\beta_i := \sup\left\{ q > 0 \mid \sum_{t=1}^{\infty} \epsilon(t)^q \pi_i(t) = +\infty \right\}.$$

The quantity β_i is called the "recurrence order" of the state i. We show that if $\epsilon(t)$ is reduced to 0 slowly enough, then

$$\eta_i - \eta_j = \beta_j - \beta_i.$$

This precisely characterizes the relationship between the time–inhomogeneous and time–homogeneous chains under slow cooling.

Next, define the "ground states" of the time–homogeneous chain as,

$$\mathcal{G} := \{ i \mid \eta_i = \min_j \eta_j \}.$$

Clearly, as $\epsilon \searrow 0$, the steady–state distribution $\{\nu_i^\epsilon\}$ gets concentrated on $\mathcal{G}$. So also, for the time–inhomogeneous chain, we show that if $\epsilon(t) \searrow 0$ slowly enough, then $x(t) \to \mathcal{G}$, in an appropriate sense. The cooling schedule $\{\epsilon(t)\}$ can then be called "quasi–static."

How fast can quasi–static cooling be? We show there exists a critical ρ^* such that $x(t) \to \mathcal{G}$ if and only if $\sum_{t=1}^{\infty} \epsilon(t)^{\rho^*} = +\infty$.

Moreover, we characterize this critical cooling rate ρ^*. It is

$$\rho^* = \max_{i \notin \mathcal{G}} \min_{i^* \in \mathcal{G}} \min_{p=(i=i_0,\ldots,i_N=i^*)} \max_{0 \le k \le N-1} (V_{i_k i_{k+1}} + \eta_{i_k} - \eta_i).$$

This critical rate is thus determined by the orders η_i. Finally, we provide a graph algorithm for computing the orders $\{\eta_i\}$, $\{\beta_i\}$, and the critical cooling rate ρ^*.

The sufficiency of slow cooling to reach the ground states has been established earlier by Chiang and Chow [8], under slightly different assumptions, and by a different procedure.

[3] More precise definitions are given in Section 3.

They also provide an algorithm to determine the rate of convergence of the occupation probabilities, under such slow cooling. Anily and Federgruen [9] have established results very similar to Theorems 6 and 7 in the context of Simulated Annealing. While their result is stronger in that they show convergence with probability one to the set of global optima, their treatment is restricted to the class of Markov chains with transition probabilties designed to optimize some objective function. The sufficient and necessary conditions obtained by them are similar to those of Theorems 6 and 7. By introducing the concept of the order of recurrence, we greatly simplify the proofs and provide a much more general treatment, although obtaining the weaker result of Cesaro convergence.

2 The Time–Homogeneous Chain, the Tree Theorem, and the Stationary Orders

Consider an irreducible, time–homogeneous Markov chain $x(t)$ on a finite state space X, with transition probabilities,

$$p_{ij} = \mathrm{Prob}(x(t+1) = j \mid x(t) = i). \tag{1}$$

Let $G(X, E(G))$ denote the underlying weighted, directed graph, which has vertex set X, arc set $E(G) = \{(i,j) \mid p_{ij} > 0 \text{ and } i \neq j\}$, and weight p_{ij} associated with each arc (i,j).

Fix a vertex i, and consider a weighted, directed, sub–graph $H(X, E(H))$ of G which satisfies,

i) every vertex $j \in X$, $j \neq i$, has exactly one arc leaving it,

ii) H contains no directed cycles,

iii) the arc weights are induced from G.

We note that such a graph is a connected tree, rooted at i. We shall say that it is an "i–graph."

Let $\mathcal{H}_i$ be the set of all such i–graphs. For any $H \in \mathcal{H}_i$, define its *weight* $w(H)$ by

$$w(H) := \prod_{(j,k)\in E(H)} p_{jk}. \tag{2}$$

The following theorem is known as the Markov Chain Tree Theorem (see [10, 11, 12, 13, 14, 15, 16]). It provides an explicit formula for the steady–state probabilities of the Markov Chain in terms of the weights $w(\cdot)$. A particularly intuitive probabilistic proof is provided in Anantharam and Tsoucas [16].

Theorem 1. *Denote by $\{\nu_i\}$ the steady–state probabilities of the Markov chain (1). Then*

$$\nu_i = \frac{\sum_{H\in\mathcal{H}_i} w(H)}{\sum_j \sum_{H\in\mathcal{H}_j} w(H)}. \tag{3}$$

We are specifically interested in the class of Markov chains whose off–diagonal transition probabilities have the form,

$$p_{ij} = c_{ij}\epsilon^{V_{ij}}, \text{ for } i \neq j. \tag{4}$$

Here $\epsilon > 0$ is a small parameter, $c_{ij} \geq 0$, and $0 \leq V_{ij} \leq +\infty$. Without loss of generality, we assume

$$V_{ij} = +\infty \Longleftrightarrow c_{ij} = 0. \tag{5}$$

Lemma 1. *Let $\{\nu_i^\epsilon\}$ denote the steady–state probabilities of the Markov chain (4). They satisfy,*

$$\nu_i^\epsilon = \Theta(\epsilon^{\alpha_i-\gamma}) \textit{ for all } i, \tag{6}$$

as $\epsilon \searrow 0$. Here

$$\alpha_i := \min_{H\in\mathcal{H}_i} \sum_{(j,k)\in E(H)} V_{jk}, \tag{7}$$

and

$$\gamma := \min_i \alpha_i. \tag{8}$$

Proof. Each p_{jk} is proportional to a power of ϵ. It follows from (2) that

$$w(H) = \left(\prod_{(j,k)\in E(H)} c_{jk}\right) \epsilon^{\sum_{(j,k)\in E(H)} V_{jk}}. \tag{9}$$

Since $c_{jk} > 0$ for all $(j,k) \in E(H)$ by (5),

$$w(H) = \Theta\left(\epsilon^{\sum_{(j,k)\in E(H)} V_{jk}}\right),$$

as $\epsilon \searrow 0$. Hence,

$$\sum_{H\in\mathcal{H}_i} w(H) = \Theta(\epsilon^{\alpha_i}),$$

and

$$\sum_j \sum_{H\in\mathcal{H}_j} w(H) = \Theta(\epsilon^{\gamma}).$$

The result follows from (3). $\square$

We will call

$$\eta_i := \alpha_i - \gamma \tag{10}$$

the *stationary order of the state* i.

Let us consider the *zero–temperature limit of the steady–state distributions*,

$$\nu_i^0 := \lim_{\epsilon\searrow 0} \nu_i^\epsilon. \tag{11}$$

The existence of the limit is guaranteed by (9) and (3). From (6), it is supported on the set of states,

$$\mathcal{G} := \{i \in X \mid \alpha_i = \min_j \alpha_j\}. \tag{12}$$

That is,

$$\sum_{i\in\mathcal{G}} \nu_i^0 = 1, \tag{13}$$

and

$$\sum_{i\in\mathcal{G}'} \nu_i^0 < 1,$$

whenever $\mathcal{G} \setminus \mathcal{G}' \neq \phi$. We will call $\mathcal{G}$ the *set of ground states* of the Markov chain (4).

3 The Time–Inhomogeneous Chain and its Recurrence Orders

We now turn to the "cooled" version of the Markov chain (4). It is a time–*inhomogeneous* Markov chain $\{x(t)\}$ with transition probabilities,

$$p_{ij}(t) = \mathrm{Prob}(x(t+1) = j \mid x(t) = i) = c_{ij}\epsilon(t)^{V_{ij}}, \text{ for } i \neq j, \tag{14}$$

where $0 < \epsilon(t) \leq 1$, while c_{ij} and V_{ij} are as before. The small parameter sequence $\{\epsilon(t)\}$ is monotone decreasing[4] and has limit 0. We call it the *cooling schedule.*

Suppose the convergence of $\epsilon(t)$ to 0 is sufficiently slow, that is, "quasi–static." Intuition suggests that this time–inhomogeneous Markov chain should converge to the set of ground states $\mathcal{G}$ of the time–homogeneous chain (4). In what follows, we will study the precise relationship between the chains (14) and (4).

We begin by defining the *order of the cooling schedule* $\{\epsilon(t)\}$ as in [6, 7].

Definition 1. *The order of the cooling schedule* $\{\epsilon(t)\}$ *is,*

$$\rho = \begin{cases} -\infty & \text{if } \sum_t \epsilon(t) < +\infty, \\ p^- & \text{if } p = \sup\{q > 0 \mid \sum_t \epsilon(t)^q = \infty\} \text{ and } \sum_t \epsilon(t)^p < +\infty, \\ p & \text{if } p = \max\{q > 0 \mid \sum_t \epsilon(t)^q = \infty\}. \end{cases}$$

The quantity ρ measures the rate of decrease of $\epsilon(t)$. The slower the cooling, the higher is ρ. We will assume throughout that

$$\rho < +\infty.$$

Let

$$\pi_i(t) := \mathrm{Prob}(x(t) = i)$$

denote the occupation probability of a state. Similar to the order of the cooling schedule, we define the *recurrence order of a state.*

[4] More generally, we only require that there exists a K such that $\epsilon(t) \leq K\epsilon(s)$ for all $0 \leq s \leq t < +\infty$.

Definition 2. *The order of recurrence, β_i, of a state i, is defined as*

$$\beta_i = \begin{cases} -\infty & \text{if } \sum_t \pi_i(t) < +\infty, \\ p^- & \text{if } p = \sup\{q > 0 \mid \sum_t \pi_i(t)\epsilon(t)^q = +\infty\} \text{ and } \sum_t \pi_i(t)\epsilon(t)^p < +\infty, \\ p & \text{if } p = \max\{q > 0 \mid \sum_t \pi_i(t)\epsilon(t)^q = +\infty\}. \end{cases}$$

This is a measure of the occupancy of the state over time. The higher the value of β_i, the more often the state i is visited.

Let

$$\mathcal{M} := \{i \in X \mid \beta_i = \max_j \beta_j\}$$

be the set of states with the largest orders of recurrence. The following Lemma, from [7], shows that the time–inhomogeneous chain converges to $\mathcal{M}$ in a Cesaro sense. To determine the asymptotic behavior of the time–inhomogeneous chain, it therefore suffices to just determine the orders of recurrence of the states, and then pick off the largest ones.

Lemma 2.

i) $\max_i \beta_i = \rho$.

ii) $\lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} \mathrm{Prob}(x(t) \in \mathcal{M}) = 1$.

The following property of *balance of recurrence orders* across cut–sets, from [6], is fundamental. Define $a \ominus b := a - b$ if $a \geq b$, and $a \ominus b := -\infty$ if $a < b$.

Theorem 2.

$$\max_{i\in A, j\in A^c} \beta_i \ominus V_{ij} = \max_{i\in A, j\in A^c} \beta_j \ominus V_{ji} \text{ for all } A \subseteq X.$$

Thus, to determine the orders of recurrence, we need to solve the set of equations,

$$\max_{i\in A, j\in A^c} \beta_i \ominus V_{ij} = \max_{i\in A, j\in A^c} \beta_j \ominus V_{ji} \text{ for all } A \subseteq X, \tag{15}$$

subject to the normalization,

$$\max_i \beta_i = \rho. \tag{16}$$

We note that at this point the difficult analytic problem of analyzing the time–inhomogeneous chain has been converted to the simpler problem of analyzing the algebraic equations (15,16). We call (15, 16) the *order balance equations.*

If ρ is large, then $\beta_i \geq V_{ij}$, see [7]. In particular, $\rho \geq 2\sum_{\{(i,j)|V_{ij}<+\infty\}} V_{ij}$ is large enough. As a result, one can replace "$\ominus$" by "$-$" in the order balance equations.

Theorem 3. *If $\rho \geq 2\sum_{\{(i,j)|V_{ij}<+\infty\}} V_{ij}$, then $\{\beta_i\}$ is the* unique *solution $\{\lambda_i\}$ of,*

$$\max_{i\in A, j\in A^c} \lambda_i - V_{ij} = \max_{i\in A, j\in A^c} \lambda_j - V_{ji} \text{ for all } A \subseteq X, \tag{17}$$

$$\max_i \lambda_i = \rho. \tag{18}$$

We will call (17, 18) the *modified order balance equations.* We will denote their solution by $\{\lambda_i\}$.

4 The Relation Between the Stationary and Recurrence Orders, and Quasi–Static Cooling

The following Theorem exhibits the relation between the stationary orders of the time–homogeneous chain, and the recurrence orders of the slowly cooled chain.

Theorem 4.

(i) The stationary orders and the solution of the modified balance equations are related by,

$$\eta_i = \rho - \lambda_i. \tag{19}$$

In particular,

$$\eta_i - \eta_j = \lambda_j - \lambda_i \text{ for all } i, j. \tag{20}$$

(ii) If the Markov chain (14) is slowly cooled, that is, ρ is large enough, then the recurrence orders $\{\beta_i\}$ are related to the stationary order $\{\eta_i\}$ by,

$$\eta_i = \rho - \beta_i.$$

Hence,

$$\eta_i - \eta_j = \beta_j - \beta_i \text{ for all } i, j.$$

In particular $\rho \geq 2 \sum_{\{(i,j) | V_{ij} < +\infty\}} V_{ij}$ *is large enough.*

Proof. The claim (ii) is a straight–forward consequence of (i), due to Theorem 3. Hence we need to only show (i).

First, consider the time–homogeneous chain (4). Let A be any subset of X. By flux balance in steady–state, i.e., $\sum_{i \in A} \sum_{j \in A^c} \nu_i^\epsilon p_{ij} = \sum_{i \in A} \sum_{j \in A^c} \nu_j^\epsilon p_{ji}$, we have

$$\sum_{i \in A} \sum_{j \in A^c} \nu_i^\epsilon c_{ij} \epsilon^{V_{ij}} = \sum_{i \in A} \sum_{j \in A^c} \nu_j^\epsilon c_{ji} \epsilon^{V_{ji}}.$$

Using (6) and equating the smallest powers of ϵ on both sides, we get

$$\min_{i \in A, j \in A^c} (\alpha_i - \gamma + V_{ij}) = \min_{i \in A, j \in A^c} (\alpha_j - \gamma + V_{ji}).$$

Hence, by (10),

$$\max_{i \in A, j \in A^c} (\rho - \eta_i) - V_{ij} = \max_{i \in A, j \in A^c} (\rho - \eta_j) - V_{ji} \text{ for every } A \subseteq X. \tag{21}$$

Moreover, by (8),

$$\max_i (\rho - \eta_i) = \rho. \tag{22}$$

Hence, $\{\rho - \eta_i\}$ satisfies the modified order balance equations (17,18). By Theorem 3, their solution is unique whenever ρ is large enough. Hence, we obtain (19). The claim (20) follows from (19). □

The same relationship between the recurrence orders of the time–inhomogeneous chain and the stationary orders of the time–homogeneous chain does not hold under rapid cooling, as the following example shows.

Example 1 Consider a Markov chain on three states, with state space $X = \{1, 2, 3\}$. See Figure 1. Let the pre–constants be $c_{13} = c_{23} = 1$, $c_{31} = 1 - \alpha$, $c_{32} = \alpha$, where $0 < \alpha < 1$, and $c_{ij} = 0$ for all other i, j. Also, suppose $V_{ij} = \max\{0, j - i\}$ for all i, j with $c_{ij} > 0$, and

$V_{ij} = +\infty$ otherwise. Let the cooling schedule be $\epsilon(t) = \frac{1}{t}$. A detailed calculation, which can be found in [17], shows that $\beta_1 = 1, \beta_2 = \alpha, \beta_3 = -\infty$. Thus, the order of recurrence β_2, of the state 2, depends on the value α of the *pre–constant* c_{32}. However, in contrast, the stationary orders for the time–homogeneous chain do *not* depend on the pre–constants. Thus, Theorem 4 does not hold for the cooling schedule $\epsilon(t) = \frac{1}{t}$. □

From Theorem 4, one deduces the *quasi–static* nature of slow cooling, that is, a slowly cooled chain converges to the set of ground states of the time–homogeneous chain.

Theorem 5. *Consider the set of ground states $\mathcal{G}$ as in (12). Then, for the time–homogeneous chain,*

$$\lim_{\epsilon \searrow 0} \sum_{i \in \mathcal{G}} \nu_i^\epsilon = 1, \tag{23}$$

while for the slowly cooled chain, with say $\rho \geq 2 \sum_{\{(i,j) \| V_{ij} < +\infty\}} V_{ij}$,

$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} \mathrm{Prob}(i \in \mathcal{G}) = 1. \tag{24}$$

Proof The result (23) follows from (13) and (11). Note that $i \in \mathcal{G}$ if and only if $i \in \mathcal{M}$. The result (24) then follows from Lemma 2.ii and Theorem 4.ii. □

5 The Circulant Algorithm for Determining the Stationary Orders

The Markov Chain Tree Theorem, Theorem 1, provides an explicit formula for the steady–state probability distribution $\{\nu_i^\epsilon\}$ of the time–homogeneous chain. However, one may only want to determine the stationary orders $\{\eta_i\}$. By (6,8), we need only compute $\{\alpha_i \mid i \in X\}$. The formula (7) provides one procedure for doing so, based on computing the minimum weights of rooted trees. An alternative procedure which exploits the connection between the η_i's and λ_i's is as follows.

From (21,22), we note that $\{-\eta_i\}$ satisfies the modified balance equations,

$$\max_{i \in A, j \in A^c} (-\eta_i - V_{ij}) = \max_{i \in A, j \in A^c} (-\eta_j - V_{ji}) \text{ for every } A \subseteq X, \tag{25}$$

subject to the normalization,

$$\max_i(-\eta_i) = 0. \tag{26}$$

Thus, the following circulant based algorithm provided in [7] for solving the modified balance equations (17,18) can be employed to determine the stationary orders $\{\eta_i\}$.

The Circulant Algorithm

Step 1. Set $A_i^1 = \{i\}$ for $i = 1, \ldots, |X|$. We call each A_i^k a coalition at step k. Let $N(1) = |X|$ be the number of coalitions at Step 1. Set $A^1 = \{A_1^1, \ldots, A_{N(1)}^1\}$.

Step k. Given $A^k = \{A_1^k, \ldots, A_{N(k)}^k\}$ where for each A_j^k the pairwise differences $\lambda_i - \lambda_j$ for states $i, j \in A_n^k$ are known (trivially for A_n^1), construct A^{k+1} as follows. Let (i_n, j_n) denote the arc (i, j) out of A_n^k which has the maximum value of $(\lambda_i - V_{ij})$. Such an arc can be deduced since the mutual differences between the λ_i's are known for all $i \in A_n^k$. Construct the directed graph $G = (V, E)$ with $V = \{A_1^k, \ldots, A_{N(k)}^k\}$ and $E = \{(i_1, j_1), \ldots, (i_{N(k)}, j_{N(k)})\}$. There is at least one directed cycle in G. If $\{A_{n_1}^k, \ldots, A_{n_p}^k\}$ is a directed cycle then $\cup_{\ell=1}^p A_{n_\ell}^k$ is defined as an element of A^{k+1}. Those elements which are not in any directed cycle are also defined as elements of A^{k+1}. Along each directed cycle we have $\lambda_i - V_{ij} = constant$. Hence, the mutual differences between λ_i and λ_j for $i, j \in A_n^{k+1}$ are determined.

Last Step. Stop when $N(k) = 1$. Since $\lambda_i - \lambda_j$ has been determined for all i, j, we have found the solution to the modified balance equations, up to a translation. $\square$

Example 2. Consider a chain with 4 states $\{1, 2, 3, 4\}$, as in Figure 2. Let the V matrix be,

$$\begin{bmatrix} * & 5 & 7 & 3 \\ +\infty & * & 4 & 7 \\ +\infty & 3 & * & 5 \\ 2 & +\infty & 7 & * \end{bmatrix}.$$

Step 1. $A^1 = \{1, 2, 3, 4\}$.

Step 2. $E = \{(1,4),(4,1),(2,3),(3,2)\}$. The two cycles formed are, $\{1,4\}$ and $\{2,3\}$. Hence,

$$\lambda_1 - 3 = \lambda_4 - 2,$$

and

$$\lambda_2 - 4 = \lambda_3 - 3.$$

Step 3. $A^2 = \{\{1,4\},\{2,3\}\}$. The arc of $\max(\lambda_i - V_{ij})$ out of $\{1,4\}$ is identified as $(1,2)$. Similarly, that out of $\{2,3\}$ is $(3,4)$. Thus, we get the cycle $\{\{1,4\},\{2,3\}\}$, and

$$\lambda_1 - 5 = \lambda_3 - 5.$$

Since $N(3) = 1$ the algorithm is terminated. Thus we have,

$$\lambda_1 - 1 = \lambda_2 - 2 = \lambda_3 - 1 = \lambda_4. \tag{27}$$

The solution of the modified balance equations has been obtained up to a translation. $\square$

The following Lemma, a corollary of Lemmas 3 and 4 of [7], will be useful in the sequel.

Lemma 3. *If $p = (i_0, i_1, \ldots, i_N)$ is a path such that $\beta_{i_n, i_{n+1}} \geq 0$ for $n = 0, 1, \ldots, N-1$, then*

$$\beta_{i_n} - \beta_{i_l} = \lambda_{i_n} - \lambda_{i_l} \text{ for } n, l \in \{0, \ldots, N\},$$

where $\{\lambda_i\}$ is the solution to the modified balance equations (17,18).

Proof. We shall denote $\beta_i \ominus V_{ij}$ by β_{ij} calling it the β–flow from i to j. Similarly, we denote $\lambda_i - V_{ij}$ by λ_{ij} and call it the λ–flow from i to j.

We use Lemma 3 of [7]. Consider the first step $k+1$ at which $i_\ell \in A_r^{k+1}$ for all $\ell = 0, \ldots, N$, for some common r. Suppose $\{A_1^k, \ldots, A_q^k\}$ is the directed cycle formed at step k for which $A_r^{k+1} = \cup_{n=1}^q A_n^k$. Since the circulant algorithm seeks arcs of maximum λ as well as β–flow at each step, the β–flow along the directed cycle $\{A_1^k, \ldots, A_q^k\}$ is non–negative. Hence, all the directed cycles within A_r^{k+1}, generated by the circulant algorithm, also have non–negative β and λ flows. It follows that the mutual differences $\beta_i - \beta_j$ for states $i, j \in A_r^{k+1}$ are the same as the mutual differences $\lambda_i - \lambda_j$. This proves the result. $\square$

Motivated by the above Lemma, we introduce the following definition.

Definition 3. *The state i is said to be recurrently connected to j if there exists a path $(i = i_0, i_1, \ldots, i_N = j)$ such that $\beta_{i_n, i_{n+1}} \geq 0$ for $0 \leq n \leq N-1$. If for every $i, j \in A$ and $k \in A^c$, i is recurrently connected to j but not to k, then A is said to be recurrently connected.*

Note that the recurrently connected sets form a partition of the state space X.

6 The Fastest Quasi–Static Cooling Rate

Consider the cooled time–inhomogeneous chain (14). In this section we determine the fastest cooling rate under which the Markov chain is still guaranteed to hit the set of ground states $\mathcal{G}$ with probability 1. Thus we determine the fastest cooling rate for quasi–static cooling.

For a state $i^* \in \mathcal{G}$, the set of ground states, and a state $i \notin \mathcal{G}$, consider paths from i to i^* of the form $p = (i = i_0, i_1, \ldots, i_N = i^*)$. Define,

$$\rho^* = \max_{i \notin \mathcal{G}} \min_{i^* \in \mathcal{G}} \min_{p=(i=i_0,\ldots,i_N=i^*)} \max_{0 \leq k \leq N-1} (V_{i_k i_{k+1}} + \lambda_i - \lambda_{i_k}). \tag{28}$$

Theorem 6 (Sufficiency). *If the order ρ of the cooling schedule satisfies $\rho \geq \rho^*$, then*

$$\lim_{T \to \infty} \frac{1}{T} \sum_{i=1}^{T} \text{Prob}(x(t) \in \mathcal{G}) = 1.$$

Proof. Suppose $\rho \geq \rho^*$. We will show that the set

$$\mathcal{M} := \{i \in X \mid \beta_i = \rho\} \subseteq \mathcal{G}. \tag{29}$$

From this, the result will follow by Lemma 2.ii.

Suppose, to the contrary, there exists a state $i \notin \mathcal{G}$ with $\beta_i = \rho$. Choose $i^* \in \mathcal{G}$ and a path $p = (i = i_0, i_1, \ldots, i_N = i^*)$ such that,

$$\max_{0 \leq k \leq N-1} (V_{i_k i_{k+1}} + \lambda_i - \lambda_{i_k}) = \min_{j^* \in \mathcal{G}} \min_{q=(i=j_0,\ldots,j_N=j^*)} \max_{0 \leq k \leq N-1} (V_{j_k j_{k+1}} + \lambda_i - \lambda_{j_k}),$$

i.e., attaining the two minima above. Then, from (28),

$$\rho \geq \rho^* \geq V_{i_k i_{k+1}} + \lambda_i - \lambda_{i_k} \text{ for } k = 0, \ldots, N-1,$$

i.e.,

$$\lambda_{i_k} - V_{i_k i_{k+1}} \geq \lambda_i - \rho \text{ for } k = 0, \ldots, N-1. \tag{30}$$

Now consider the β–flow along the path p. Suppose there exists a k such that

$$\beta_{i_k} - V_{i_k i_{k+1}} < 0, \tag{31}$$

but

$$\beta_{i_l} - V_{i_l i_{l+1}} \geq 0 \text{ for } l = 0, \ldots, k-1.$$

Then applying Lemma 3 to the path $(i = i_0, i_1, \ldots, i_k)$, we obtain

$$\begin{aligned} \beta_{i_k} &= \lambda_{i_k} - \lambda_i + \beta_i \\ &= \lambda_{i_k} - \lambda_i + \rho. \end{aligned}$$

Hence,

$$\begin{aligned} \beta_{i_k} - V_{i_k i_{k+1}} &= (\lambda_{i_k} - V_{i_k i_{k+1}}) - (\lambda_i - \rho) \\ &\geq 0, \qquad \text{(from (30))}. \end{aligned}$$

This contradicts (31).

Thus, we have $\beta_{i_k i_{k+1}} \geq 0$ for $k = 0, \ldots, N-1$. Applying Lemma 3 again, this time to the entire path $p = (i = i_0, \ldots, i_N = i^*)$, we obtain,

$$\begin{aligned} \beta_{i^*} &= \lambda_{i^*} - \lambda_i + \beta_i \\ &= \alpha_i - \alpha_{i^*} + \beta_i \qquad \text{(from (20))} \\ &> \beta_i \qquad \text{(since } i^* \in \mathcal{G} \text{ but } i \notin \mathcal{G} \text{ from (14))} \\ &= \rho. \end{aligned}$$

This is a contradiction to Lemma 2.i.

Thus there cannot exist a state $i \notin \mathcal{G}$ with $\beta_i = \rho$. This proves (29), concluding the proof. □

Remark 1. In seeking the minimum over $i^* \in \mathcal{G}$ and paths $p = (i = i_0, \ldots, i_N = i^*)$ in (28), it suffices to consider the earliest step k at which a coalition A_l^k containing i also intersects $\mathcal{G}$. The resulting $i^* \in A_l^k \cap \mathcal{G}$, and the resulting path p which is a part of the directed cycle at that step, attain the minima in (28). This reduces the computational burden in computing ρ^*.

Theorem 7 (Necessity). *If $\rho < \rho^*$, then there exists an initial state $x(0) = i_0 \in X$ such that,*

$$\mathrm{Prob}(x(t) \notin \mathcal{G}, \ \ \forall t \geq 0) > 0.$$

Proof. Suppose $\rho < \rho^*$. From (28), this means there exists a state, say $i_0 \notin \mathcal{G}$, such that for every path $p = (i_0, i_1, \ldots, i_N)$ with $i_N \in \mathcal{G}$, $\rho < \max_{0 \leq N-1}(V_{i_k i_{k+1}} + \lambda_{i_0} - \lambda_{i_k})$. Hence, for every path there exists an n such that $\rho - V_{i_m i_{m+1}} - \lambda_{i_0} + \lambda_{i_m} \geq 0$ for all $m = 0, 1, \ldots, n-1$, while $\rho - V_{i_n i_{n+1}} - \lambda_{i_0} + \lambda_{i_n} < 0$.

Suppose i_0 is recurrently connected to i_n. Then by Lemma 3,

$$\begin{aligned} \beta_{i_n} - V_{i_n i_{n+1}} &= \beta_{i_0} + \lambda_{i_n} - \lambda_{i_0} - V_{i_n i_{n+1}} \\ &\leq \rho + \lambda_{i_n} - \lambda_{i_0} - V_{i_n i_{n+1}} \\ &< 0, \end{aligned}$$

and so $\beta_{i_n i_{n+1}} = -\infty$. So i_0 cannot be recurrently connected to i_N. Thus, if Y is the recurrently connected set containing i_0, then $Y \cap \mathcal{G} = \phi$.

Consider another set Y' with the same number of elements as Y. Associate each state $i \in Y$ uniquely with a state $i' \in Y'$.

We now construct a new Markov chain $\{\tilde{x}(t)\}$ on the state space $Y \cup Y'$, with transition probabilities given by,

$$\begin{aligned} \tilde{p}_{ij}(t) &:= p_{ij}(t) \text{ for all } i, j \in Y, \\ \tilde{p}_{i'j}(t) &:= p_{ij}(t) \text{ for all } i' \in Y', \ \ j \in Y, \\ \tilde{p}_{jj'}(t) &:= \sum_{k \notin Y} p_{jk}(t) \text{ for all } j \in Y, \ \ j' \in Y', \end{aligned}$$

where the $p_{ij}(t)$'s are as in (14). We choose the initial state $\tilde{x}(0) = x(0)$ in Y.

For $j \in Y$, let us denote $\min_{k \notin Y} V_{jk}$ by $V_{jj'}$. Note that $V_{jj'} > 0$, since Y is recurrently connected. We note that for any $j \in Y$, $j' \in Y'$,

$$c_1 \epsilon(t)^{V_{jj'}} \leq \tilde{p}_{jj'}(t) \leq c_2 \epsilon(t)^{V_{jj'}},$$

for some $c_1, c_2 > 0$. By Remark 2.5 of [6], our theory also applies to the chain $\{\tilde{x}(t)\}$.

Now we compare the running of the circulant algorithm on the chains $\{x(t)\}$ and $\{\tilde{x}(t)\}$. Focus on states in Y. We see that at the same step k, one will have $A_l^k = Y$ in both algorithms. Thus the mutual differences in the recurrence orders for the states in Y are the same for both the chains.

Note also that

$$\mathrm{Prob}(\tilde{x}(t+1) = j') \leq c_2 \mathrm{Prob}(\tilde{x}(t) = j)\ \epsilon(t)^{V_{jj'}}.$$

Since $V_{jj'} > 0$, the recurrence order of j' is strictly less than that of j. Hence, no state in Y' can have the *maximum* order of recurrence. Denoting the recurrence orders for $\{\tilde{x}(t)\}$ by $\tilde{\beta}_i$, we thus have $\tilde{\beta}_i = \rho$ for some $i \in Y$. Hence, the recurrence order of i in $\{\tilde{x}(t)\}$ is larger than or equal to that in $\{x(t)\}$.

Since the mutual differences of the recurrence orders agree for both chains for all states in Y, and their maximum values are equal, it follows that $\beta_i = \tilde{\beta}_i$ all states in Y.

Hence, all states in Y are recurrently connected to all other states in Y, in $\{\tilde{x}(t)\}$.

Note that $\beta_j - V_{jk} < 0$ for all states $j \in Y, k \notin Y$ for the original chain $\{x(t)\}$. Hence, $\beta_j - V_{jj'} < 0$ for all $j \in Y$ for the new chain $\{\tilde{x}(t)\}$. It follows that Y is a recurrently connected set in $\{\tilde{x}(t)\}$. So,

$$\sum_{t=1}^{\infty} \mathrm{Prob}(\tilde{x}(t) = j, \tilde{x}(t+1) = j') < +\infty \text{ for all } j \in Y \text{ and corresponding } j' \in Y'.$$

By the Borel–Cantelli lemma, it follows that the transition $j \to j'$ occurs only finitely many times with probability one. That is, there is a time T, and a state $j^* \in Y$, such that

$$\mathrm{Prob}(\tilde{x}(T) = j^*,\ \ \tilde{x}(t) \in Y\ \ \forall t > T) > 0.$$

This means that,

$$\mathrm{Prob}(\tilde{x}(T) = j^*) \;\; \mathrm{Prob}(\tilde{x}(t) \in Y \;\; \forall t > T \mid \tilde{x}(T) = j^*) > 0,$$

and in particular that,

$$\mathrm{Prob}(\tilde{x}(t) \in Y \;\; \forall t > T \quad \mid \tilde{x}(T) = j^*) > 0.$$

Note that $\tilde{x}(0) = x(0)$. Since $p_{ij}(t) = \tilde{p}_{ij}(t)$ for states $i, j \in Y$, we have

$$\mathrm{Prob}(x(t) \in Y \;\; \forall t > T \mid x(T) = j^*) = \mathrm{Prob}(\tilde{x}(t) \in Y \;\; \forall t > T \mid \tilde{x}(T) = j^*) > 0. \tag{32}$$

Now choose an initial condition $x(0) = j_0$ and a sequence $\{j_1, j_2, \ldots, j_{T-1}, j_T = j^*\}$, with $j_i \in Y$ for $0 \leq i \leq T-1$ such that

$$\mathrm{Prob}(x(t) = j_t, \;\; 1 \leq t \leq T \mid x(0) = j_0) > 0. \tag{33}$$

There always exists such a choice.

From (32,33)

$$\mathrm{Prob}(x(t) \in Y \;\; \forall t \geq 1 \mid x(0) = j_0) > 0.$$

This proves the Theorem. □

Example 2 (Continued). Consider the same chain as in Example 2. We already know that

$$\lambda_1 - 1 = \lambda_2 - 2 = \lambda_3 - 1 = \lambda_4.$$

Thus $\lambda_2 > \max(\lambda_1, \lambda_3, \lambda_4)$, and so $\mathcal{G} = \{2\}$. Using Remark 1 to economize the computation, we note the following.

(i) States 3 and $i^* = 2$ fall into the same coalition at step 2, and so from (28) we have $\rho^* \geq V_{32} = 3$.

(ii) States 1 and $i^* = 2$ fall into the same coalition at step 3, and so we have $\rho^* \geq V_{12} = 5$.

(iii) States 4 and $i^* = 2$ fall into the same coalition at step 3. Here we have the path $p = (4, 1, 2)$ connecting states 4 and 2. Along the arc $(4, 1)$ we require $\rho^* \geq 2$ and along the arc $(1, 2)$ we require $\rho^* \geq (V_{12} - \lambda_1 + \lambda_4) = 4$.

The smallest value of ρ^* meeting the above requirements is 5. So we conclude that $\rho^* = 5$. If the cooling rate is less than 5, there is a non–zero probability that the chain never reaches state 2, if it starts in state $x(0) = 1$ or $x(0) = 4$ (or even $x(0) = 3$). □

7 Simulated Annealing

Consider the method of optimization by simulated annealing. There, one has a cost W_j for every state $j \in X$. The goal is to determine a global minimum of W. The choice

$$V_{ij} = (W_j - W_i)^+ \text{ for } j \in \text{Neighborhood of } i, \tag{34}$$

is popular.

However, the ground states are determined not just by $\{V_{ij}\}$, but also by the choice of the *neighborhoods*. In the following example, the asymmetric choice of neighborhood structure results in the ground states being different from the global minima of W.

Example 3. Consider the three state chain on $X = \{1, 2, 3\}$. See Figure 3. Let $W_1 = 1$, $W_2 = 2$ and $W_3 = 4$, $c_{12} = c_{23} = c_{31} = 1$, and all other c_{ij} equal to zero. The V_{ij} are $V_{12} = (W_2 - W_1)^+ = 1$, $V_{23} = (W_3 - W_2)^+ = 2$ and $V_{31} = (W_1 - W_3)^+ = 0$. Note that even though the transition $1 \to 2$ is possible, the reverse transition is not. Hence, the neighborhoods are not "symmetric."

The modified balance equations are,

$$\lambda_1 - 1 = \lambda_2 - 2 = \lambda_3.$$

This shows that the set of ground states is $\mathcal{G} = \{2\}$. It differs from the global minimum set $\{1\}$ of W. The critical cooling rate is $\rho^* = 1$. When quasi–statically cooled with $\rho \geq 1$, the process anneals to the state 2 rather than 1. □

Let us therefore make the symmetric neighborhood assumption,

$$c_{ij} > 0 \Leftrightarrow c_{ji} > 0.$$

From [7], we have

$$\lambda_i + W_i = \text{ constant for all } i. \tag{35}$$

Hence, the set of ground states is

$$\mathcal{G} = \{i \mid W_i = \min_j W_j\}.$$

It coincides with the set of global minima, as desired.

From (35,34), we also have

$$\begin{aligned} \rho^* &= \max_{i \notin \mathcal{G}} \min_{i^* \in \mathcal{G}} \min_{p=(i=i_0,\ldots,i_N=i^*)} \max_{0 \le k \le N-1} ((W_{i_{k+1}} - W_{i_k})^+ + W_{i_k} - W_i) \\ &= \max_{i \notin \mathcal{G}} \min_{i^* \in \mathcal{G}} \min_{p=(i=i_0,\ldots,i_N=i^*)} \max_{0 \le k \le N-1} (W_{i_k} - W_i). \end{aligned} \tag{36}$$

This is simply the minimum height necessary to be surmounted, when seeking paths from states in $\mathcal{G}$ to a global minimum state.

Consider now the more general assumption of "weak reversibility" of [4]. Still, the same result (35) continues to hold, as shown in [7]. Hence, the critical cooling rate ρ^* continues to be given by (36). Such a critical cooling rate has been obtained by Hajek [4], who has shown convergence in probability to the set of global minima if $\rho \ge \rho^*$.

8 Concluding Remarks

We have obtained the exact connection between slowly cooled Markov chains, and the family of time–homogeneous chains. We have determined the precise relationship between certain state occupancy measures for both chains. When the cooling is slow, the time–inhomogeneous chain converges to the set of ground states of the time–homogeneous chains. We have determined the critical cooling rate for such quasi–static cooling. Finally, we have provided a graph algorithm to determine the measures of occupancy as well as the critical cooling rate.

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