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Structure and eigenvalues of heat-bath Markov chains

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We prove that heat-bath chains (which we define in a general setting) have no negative eigenvalues. Two applications of this result are presented: one to single-site heat-bath chains for spin systems and one to a heat-bath Markov chain for sampling contingency tables. Some implications of our main result for the analysis of the mixing time of heat-bath Markov chains are discussed. We also prove an alternative characterisation of heat-bath chains, and consider possible generalisations.

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1. Definitions and our first result

Suppose that Ω is a finite set and let $\pi : \Omega \to (0, 1]$ be a probability distribution on Ω. Let $\mathcal{L}$ be a nonempty finite index set and let $L = |\mathcal{L}|$. Suppose that for all $x \in \Omega$ and $a \in \mathcal{L}$ we have a subset $\Omega_{x,a}$ of Ω such that

(I) $x \in \Omega_{x,a}$ for all $x \in \Omega$ and $a \in \mathcal{L}$, and
(II) for each $a \in \mathcal{L}$, the set $\{\Omega_{x,a} : x \in \Omega\}$ forms a partition of Ω.

For $a \in \mathcal{L}$, define the $|\Omega| \times |\Omega|$ matrix P_a (with rows and columns indexed by Ω) by

$$P_a(x, y) = \frac{\pi(y)}{\pi(\Omega_{x,a})} \mathbb{1}(y \in \Omega_{x,a}). \tag{1}$$

(Here $\mathbb{1}(y \in \Omega_{x,a})$ equals 1 if $y \in \Omega_{x,a}$, and equals 0 otherwise.) Note that P_a is well-defined for all $a \in \mathcal{L}$, since π is nonzero on all states and each set $\Omega_{x,a}$ is nonempty.

Now for a given probability distribution ρ on $\mathcal{L}$, let P be the $|\Omega| \times |\Omega|$ matrix defined by

$$P = \sum_{a \in \mathcal{L}} \rho(a) P_a. \tag{2}$$

Since P is a stochastic matrix, it defines a Markov chain $\mathcal{M}$ on Ω, determined uniquely by π, $\mathcal{L}$, ρ, and the sets $\Omega_{x,a}$. A transition of $\mathcal{M}$ from current state $x \in \Omega$ is performed by choosing an element $a \in \mathcal{L}$ according to the distribution ρ, then sampling the next state y from $\Omega_{x,a}$ with respect to the distribution π restricted to $\Omega_{x,a}$.

Definition 1.1. A Markov chain $\mathcal{M}$ on a finite state space Ω is a *heat-bath chain* if its transition matrix P satisfies (2) with respect to some finite nonempty set $\mathcal{L}$ equipped with a probability distribution ρ, some probability distribution $\pi : \Omega \to (0, 1]$, and some sets $\Omega_{x,a}$ which satisfy (I), (II). Here the matrices P_a in (2) are defined by (1).

Note that conditions (I) and (II) imply that for all $x, y \in \Omega$ and $a \in \mathcal{L}$,

$$\text{if } y \in \Omega_{x,a} \quad \text{then } \Omega_{x,a} = \Omega_{y,a}. \tag{3}$$

Furthermore, when (2) holds it follows that $\mathcal{M}$ is aperiodic (since every state has a self-loop) and that $\mathcal{M}$ is reversible with respect to π. However, the chain $\mathcal{M}$ need not be irreducible. (See [11] for Markov chain definitions which are not given here.)

Before proceeding, we indicate how our definition of heat-bath chains corresponds to the usual notion of heat-bath chains, in the setting of graph colourings or the Potts model. In such a chain, the state space is a subset of S^V for some finite sets V, S. To express this using our formulation, let $\mathcal{L} = \{a_1, \ldots, a_L\}$ be the set of all those subsets $a_i \subset V$ which may be updated by a single transition of the chain, and, for $a \in \mathcal{L}$,