

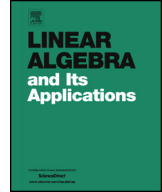


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## Structure and eigenvalues of heat-bath Markov chains



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### ABSTRACT

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  $\Omega$  is a finite set and let  $\pi : \Omega \rightarrow (0, 1]$  be a probability distribution on  $\Omega$ . 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  $\Omega$  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  $\Omega$ .

For  $a \in \mathcal{L}$ , define the  $|\Omega| \times |\Omega|$  matrix  $P_a$  (with rows and columns indexed by  $\Omega$ ) 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  $\pi$  is nonzero on all states and each set  $\Omega_{x,a}$  is nonempty.

Now for a given probability distribution  $\rho$  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  $\Omega$ , determined uniquely by  $\pi$ ,  $\mathcal{L}$ ,  $\rho$ , 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  $\rho$ , then sampling the next state  $y$  from  $\Omega_{x,a}$  with respect to the distribution  $\pi$  restricted to  $\Omega_{x,a}$ .

**Definition 1.1.** A Markov chain  $\mathcal{M}$  on a finite state space  $\Omega$  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  $\rho$ , some probability distribution  $\pi : \Omega \rightarrow (0, 1]$ , 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  $a \in \mathcal{L}$ ,

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

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  $\pi$ . 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  $\mathcal{L} = \{a_1, \dots, a_L\}$  be the set of all those subsets  $a_i \subset V$  which may be updated by a single transition of the chain, and, for  $a \in \mathcal{L}$ ,

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