University of Jyväskylä
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MATS255 Markov Processes

Exercise 6
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Gibbs sampler for random hardcore configurations

Let $G = (V, E)$ be a finite undirected graph with vertices $V = \{v_1, \dots, v_k\}$ and edges $E = \{e_1, \dots, e_\ell\}$. Denote by $\{0,1\}^V$ the set of functions from V into $\{0,1\}$. An element $\xi \in \{0,1\}^V$ is called a *configuration*, and we say that a vertex v is occupied if $\xi(v) = 1$ and vacant otherwise. An element $\xi \in \{0,1\}^V$ is called a feasible hardcore configuration on G if no neighboring vertices of G are occupied. We denote the set of feasible configurations by

$$S = \{\xi \in \{0,1\}^V : \xi(v) + \xi(w) \le 1 \text{ for all } (v,w) \in E\}.$$

Construct a Markov chain (X_n) on S recursively (as in [Häg02, Example 7.2]) by letting X_0 be an arbitrary feasible configuration on G, and at each integer time $n+1$:

1. Pick a vertex $v \in V$ uniformly at random.
2. Toss a fair coin.
3. If the coin comes up heads, and all neighbors of v take value 0 in X_n, then let $X_{n+1}(v) = 1$; otherwise let $X_{n+1}(v) = 0$.
4. For all vertices w other than v, leave the value at w unchanged, i.e., let $X_{n+1}(w) = X_n(w)$.

6.1 Write down the transition matrix P of (X_n), and convince yourself (and others) that this random process really is a Markov chain.

6.2 Show that the uniform distribution on S is reversible for (X_n). Can you find a simple proof of this fact using a simple structural property of P?

6.3 Show that (X_n) is aperiodic.

6.4 Show that (X_n) is irreducible. (**Hint:** Show first that the empty configuration can be reached from any feasible configuration in a finite number of steps.)

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Boltzmann distribution at a low temperature

6.5 Let S be a finite set and let $f : S \to \mathbb{R}$ be arbitrary. The *Boltzmann distribution* $\pi_{f,T}$ with energy f and temperature T is the probability vector

$$\pi_{f,T}(s) = Z_{f,T}^{-1} e^{-f(s)/T},$$

where the normalizing constant is given by $Z_{f,T} = \sum_{s \in S} e^{-f(s)/T}$. Let Y be a random variable having the Boltzmann distribution $\pi_{f,T}$. Show that

$$\mathbb{P}\left(f(Y) = \min_{s \in S} f(s) \right) \to 1 \quad \text{as } T \to 0.$$

St. Lucy's Day bonus problems

6.6* *General Metropolis chain.* (*Worth 1 exercise point*). [LPW09, Ex 3.1] Let Ψ be an irreducible transition matrix on a finite state space S, and let π be a probability vector on S such that $\pi_i > 0$ for all $i \in S$. Show that the transition matrix

$$P_{i,j} = \begin{cases} \Psi_{i,j} \min(\frac{\pi_j \Psi_{j,i}}{\pi_i \Psi_{i,j}}, 1), & \text{if } j \neq i, \\ 1 - \sum_{\ell \neq i} \Psi_{i,\ell} \min(\frac{\pi_\ell \Psi_{\ell,i}}{\pi_i \Psi_{i,\ell}}, 1) & \text{if } j = i, \end{cases}$$

defines a reversible Markov chain with stationary distribution π.

6.7** *Gibbs sampler for random chessboard kings.* (*Worth 2 exercise points*). Let G be a graph where vertices correspond to chessboard squares, and where vertices v and w are connected if a king can go from v to w in one move. Write a program which simulates a (uniformly) randomly chosen feasible hardcore configuration on G using the Gibbs sampler described above.

(a) Draw a realization of $f(X_n)$, where $f(\xi) = \sum_{v \in V} \xi(v)$ is the number of particles in configuration ξ.

(b) Estimate numerically the mean number of particles in a uniformly random chosen feasible configuration.

References

[Häg02] Olle Häggström. *Finite Markov chains and Algorithmic Applications.* Cambridge University Press, 2002.

[LPW09] David A. Levin, Yuval Peres, and Elizabeth L. Wilmer. *Markov Chains and Mixing Times.* American Mathematical Society, 2009.