Key Solution For problem 8.5, 8.4

Chapter 8: Markov Chain Monte Carlo Methods - Solutions to Selected problems

8.4 Let $G = (V, E)$ be an undirected, connected graph with the property that each vertex is connected to at most r vertices. Let f be a positive function defined on V and let π denote the probability distribution

$$\pi(x) = \frac{f(x)}{\sum_{v \in V} f(v)} .$$

If $(x, y) \in E$, define the transition probability

$$p(x, y) = \frac{1}{r} min \left\{ 1, \frac{f(y)}{f(x)} \right\} .$$

with $p(x, y) = 0$ otherwise, except that $p(x, x)$ is determined so that the rows sum to one. (i) Show that the Markov chain determined by p is irreducible. (ii) Determine conditions under which the chain is regular. (iii) Show the chain is time reversible with respect to π.

Solution (i) To show that the chain is irreducible, note first that G is connected. In other words, in G there is a path from any one node to any other; that is, given any two nodes, say a and b in V, there is a sequence of nodes, say $x_1, x_2, \cdots, x_n$, in V such that $(a, x_1) \in E$, $(x_i, x_{i+1}) \in E$, for each $i = 1, 2, \cdots, n$, and $(x_n, b) \in E$. While the graph G is undirected, the graph of the Markov chain is directed. However, corresponding to each arc in G there are two arcs in the graph of the Markov chain, one in each direction, and each with nonzero probability. Indeed, if $(x, y) \in E$, then there is an arc in the graph of the Markov chain that points from x to y with associated probability $p(x, y) > 0$, determined by the formula above, and there is another arc that points from y to x with associated probability $p(y, x) > 0$, again determined by the formula above. It follows that in the graph of the Markov chain, between any two nodes (now states of the chain), there is a path between these states that can be traversed following the arcs in the required directions. In other words, any two states of the Markov chain communicate. Hence, the chain is irreducible.

(ii) Although the Markov chain is irreducible, it may be periodic, and hence not regular. As a simple example, consider the graph $G = (V, E)$ with vertex set $V = \{1, 2\}$ and edge set $E = \{(1, 2)\}$. Then $r = 1$. Suppose that f is the constant function. Then the associated Markov chain has one-step probability transition matrix

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} .$$

This chain is periodic with period 2. Suppose however that f is not constant. For example, let $f(1) = 1$ and $f(2) = 3$. Then the associated Markov chain has one-step probability transition matrix

$$P = \begin{bmatrix} 0 & 1 \\ 1/3 & 2/3 \end{bmatrix} .$$

This chain is aperiodic. However, more generally, whenever f is not the constant function, the associated Markov chain will be aperiodic, and hence regular. To see this result, note that there must be some vertex x such that $(x, y) \in E$, and $f(y) < f(x)$. For this state x, the sum of the off-diagonal elements will be less than one, since there are at most r nonzero off diagonal entries. Hence, for this row, $p(x, x) \neq 0$. Thus, state x is aperiodic, and since the chain is irreducible, all states are aperiodic, and so the chain is aperiodic.

As another condition which implies regularity, suppose that at least one node of the graph G is connected directly to fewer than r nodes. Then, whether f is the constant function or not, that node will become a state in the chain that is aperiodic. Indeed, in the one-step transition matrix, the row corresponding to this state will be such that the sum of the off-diagonal elements will be less than one, and hence the diagonal element will be nonzero. Thus, since the chain is irreducible, and one state is aperiodic, all states are aperiodic.

(iii) To show that the balance equations hold, we need to show that $\pi(x)p(x, y) = \pi(y)p(y, x)$ for each pair of states x and y. First, if $p(x, y) = 0$, then $p(y, x) = 0$ also, since $p(x, y) = 0$ only when there is no edge of the graph G that connects x and y. Next, when $(x, y) \in E$,

$$\pi(x)p(x, y) = \frac{f(x)}{rC} min \left\{ 1, \frac{f(y)}{f(x)} \right\} = \frac{1}{rC} min \left\{ f(x), f(y) \right\} ,$$

where C is the sum appearing in the denominator of π. Similarly, we have

$$\pi(y)p(y, x) = \frac{f(y)}{rC} min \left\{ 1, \frac{f(x)}{f(y)} \right\} = \frac{1}{rC} min \left\{ f(y), f(x) \right\} ,$$

These two expressions are the same, which is the desired conclusion.

8.5 Suppose $G = (V, E)$ is an undirected connected graph. For each vertex $v \in V$, let $edge(v)$ denote the number of edges that are connected to v. Let f be a positive function defined on V, and letπ denote the probability distribution

$$\pi(x) = \frac{f(x)}{\sum_{v \in V} f(v)} .$$

(a) Implement the Hastings-Metropolis method to find a regular Markov chain whose limiting distribution is π. Start with the initial irreducible chain defined by

$$q(x, y) = \frac{1}{edge(x)} , \quad \text{whenever} \quad (x, y) \in E .$$

Note that the Markov chain with this one-step transition matrix is traversed by selecting at random one of the edges connected to x, and then making the transition to the corresponding node. $(a1)$ Show that the Markov chain determined by this method is irreducible. $(a2)$ Determine conditions under which the chain is regular. $(a3)$ Show the chain is time reversible with respect to π. (b) Write a MATLAB program that determines the one-step probability matrix resulting from this method. The input to this program is the function f and the graph, represented by an adjacency matrix. An adjacency matrix is an $n \times n$ matrix, where n is the number of nodes in the graph, and where entry (i, j) is one if there is an edge connecting nodes i and j, and is zero otherwise. Use this adjacency matrix to compute the function $edge(v)$ at each node. Apply your program to the graph $G = (V, E)$ where $V = \{1, 2, 3, 4\}$, and $E = \{(1, 2), (1, 3), (2, 3), (2, 4), (3, 4)\}$, and where $f(1) = 2$, $f(2) = 8$, $f(3) = 6$, and $f(4) = 4$. Verify (using MATLAB) that the resulting chain is regular and has the required limiting state probability distribution.

Solution (a) The one-step transition probabilities are

$$p(x,y) = \frac{1}{edge(x)}\beta(x,y) \quad \text{for } (x,y) \in E \,, \quad \text{with } p(x,x) = 1 - \sum_{y \neq x} p(x,y) \,,$$

where $\beta(x, y)$ is given by

$$\beta(x,y) = min\left\{1, \frac{f(y)edge(x)}{f(x)edge(y)}\right\} \,.$$

Otherwise $p(x, y) = 0$.

$(a1)$ These formulas show that for each arc $(x, y) \in E$, we have $p(x, y) > 0$ and $p(y, x) > 0$. Thus, between any two nodes that are connected by an arc in G, the resulting Markov chain has two corresponding states, x and y, and there are two arcs connecting these states which point in opposite directions. Hence, since the original graph is connected, it is therefore possible, in the Markov chain, to travel from any one state to any other. Thus, the chain is irreducible.

$(a2)$ For the setting of this problem, the Markov chain produced by the Hasting-Metropolis algorithm may be periodic, and hence not regular. For example, consider the graph $G = (V, E)$ with vertex set $V = \{1, 2\}$ and edge set $E = \{(1, 2)\}$. Suppose that f is the constant function. Then the resulting Markov chain has one-step probability transition matrix

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} ,$$

and the chain is periodic with period 2.

However, when $f(x)/edge(x)$ is not the constant function on V, the chain is aperiodic. To see this result, note first that since the graph is connected, there must be two vertices x and y such that $(x, y) \in E$, and $f(y)/edge(y) < f(x)/edge(x)$. For these states x and y we will have $\beta(x, y) < 1$. Therefore, in the one step transition matrix for the Markov chain, the sum of the off-diagonal elements in the row for state x is less than one. Hence, state x is aperiodic. Since the chain is irreducible, the chain is therefore also aperiodic. Thus, in this case when $f(x)/edge(x)$ is not the constant function on V, the chain is irreducible and aperiodic, and hence regular.

$(a3)$ To show that the balance equations hold, the same argument used for the previous problem carries over. we need to show that $\pi(x)p(x, y) = \pi(y)p(y, x)$ for each pair of states x and y. First, if $p(x, y) = 0$, then $p(y, x) = 0$ also, since $p(x, y) = 0$ only when there is no edge of the graph G that connects x and y. Next, when $(x, y) \in E$,

$$\pi(x)p(x, y) = \frac{f(x)}{edge(x)C} min\left\{1, \frac{f(y)edge(x)}{f(x)edge(y)}\right\} = \frac{1}{C} min\left\{\frac{f(x)}{edge(x)}, \frac{f(y)}{edge(y)}\right\},$$

where C is the sum appearing in the denominator of π. Similarly, we have

$$\pi(y)p(y, x) = \frac{f(y)}{edge(y)C} min\left\{1, \frac{f(x)edge(y)}{f(y)edge(x)}\right\} = \frac{1}{C} min\left\{\frac{f(y)}{edge(y)}, \frac{f(x)}{edge(x)}\right\},$$

These two expressions are the same, which is the desired conclusion.