TMA4300 Computer Intensive Statistical Methods
Interactive lecture 3, Spring 2018

Problem A: Markov chain Monte Carlo for a toy problem

Consider a discrete distribution $f_X(x), x \in \{0,1\}$, where $f_X(1) = \alpha$ and $f_X(0) = 1 - \alpha$ for some $\alpha \in (0,1)$. Of course we know how to simulate from such a distribution directly, but in this problem we will still consider how we can simulate from this distribution by simulating a Markov chain with limiting distribution $f_X(x)$.
Let $P(y|x), x, y \in \{0,1\}$ be the transition matrix of a Markov chain on $\{0,1\}$. We then know that $f_X(x)$ is a stationary distribution for the Markov chain if

$$\sum_{x=0}^{1} f_X(x)P(y|x) = f_X(y) \quad \text{for } y \in \{0,1\}. \tag{1}$$

If the chain is irreducible and aperiodic, $f_X(x)$ is also the unique limiting distribution of the Markov chain.

1. Characterise all transition matrices $P(y|x)$ that has limiting distribution $f_X(x)$.
2. Implement a function in R that simulates a Markov chain with limiting distribution $f_X(x)$ for a specified number of steps and returns the whole simulated Markov chain.
3. Run your R function many times and use the output to estimate the distribution of the state of the Markov chain after i steps, for different values of i. How many iterations was necessary for your Markov chain to have converged to the limiting distribution?
4. Discuss how you can choose the transition matrix $P(y|x)$ to obtain a Markov chain with very fast convergence? What transition matrix would give very slow convergence? Check that you have found reasonable answers by simulating and monitoring the convergence as above.

Problem B: Markov chain Monte Carlo and time reversibility

Consider a discrete distribution $f(x), x \in \Omega = \{1, \dots, n\}$ (to simplify the notation we are now omiting the subscript X). Of course we again know how to simulate from this distribution, but we will still consider how simulate from it by Markov chain Monte Carlo. A Markov chain with transition matrix $P(y|x), x, y \in \Omega$ has stationary distribution $f(x)$ if

$$\sum_{x \in \Omega} f(x) P(y|x) = f(y) \quad \text{for all } y \in \Omega. \tag{2}$$

If the chain is irreducible and aperiodic, $f(x)$ is also the unique limiting distribution.

1. A Markov chain with transition matrix $P(y|x)$ is said to be time reversible if

$$f(x)P(y|x) = f(y)P(x|y) \quad \text{for all } x, y \in \Omega. \tag{3}$$

   Show that (3) implies (2).

In the following we set $n = 3$, $f(1) = 0.1$, $f(2) = 0.4$ and $f(3) = 0.5$.

2. Find one transition matrix $P(y|x)$ so that the resulting Markov chain has limiting distribution $f(x)$.

3. If the transition matrix you found in 2 defines a time reversible Markov chain, find another transition matrix which defines a Markov chain which is not time reversible and has limiting distribution $f(x)$. If the transition matrix you found in 2 defines a Markov chain which is not time reversible, find another transition matrix which defines a time reversible Markov chain with limiting distribution $f(x)$.

4. For each of the two transition matrices found above, implement an R function which simulates the Markov chain for a specified number of iterations and returns the last state. Check numerically that the two Markov chains you have defined have the correct limiting distribution.

5. Let $P_1(y|x)$ and $P_2(y|x)$ denote the transition matrices you defined in 2 and 3, respectively. Use these to define a new transition matrix

$$P_3(y|x) = pP_1(y|x) + (1-p)P_2(y|x), \tag{4}$$

   where $p \in (0, 1)$. How can you simulate a Markov chain with transition matrix $P_3(y|x)$? Implement an R function that simulates the Markov chain defined by $P_3(y|x)$ with a specified number of iterations and returns the last state. The parameter p should be an input parameter in the R function. Estimate the limiting distribution of this new Markov chain by calling your R function many times. How does the limiting distribution compare with $f(x)$?

6. Define a transition matrix $P_4(y|x)$ by

$$P_4(y|x) = \sum_{z \in \Omega} P_1(z|x) P_2(y|z). \tag{5}$$

How can you simulate a Markov chain with transition matrix $P_4(y|x)$? Implement an R function that simulates the Markov chain defined by $P_4(y|x)$ with a specified number of iterations and returns the last state. The parameter p should be an input parameter in the R function. Estimate the limiting distribution of this new Markov chain by calling your R function many times. How does the limiting distribution compare with $f(x)$?

In the last item of this problem we again consider the general distribution $f(x), x \in \{1, 2, \ldots, n\}$.

5. Assume each of $P_1(y|x)$ and $P_2(y|x)$ are transition matrices that fulfil (2) and define $P_3(y|x)$ and $P_4(y|x)$ as in (4) and (5), respectively. Show analytically that then also $P_3(y|x)$ and $P_4(y|x)$ fulfil (2).