5 Various types of Markov chains

In this exercise you will practice your skills learned so far by analyzing various different types of Markov chains. You get introduced to the notion of reversibility. You also get introduced to the famous Metropolis algorithm that is widely used in Markov chain Monte Carlo algorithms.

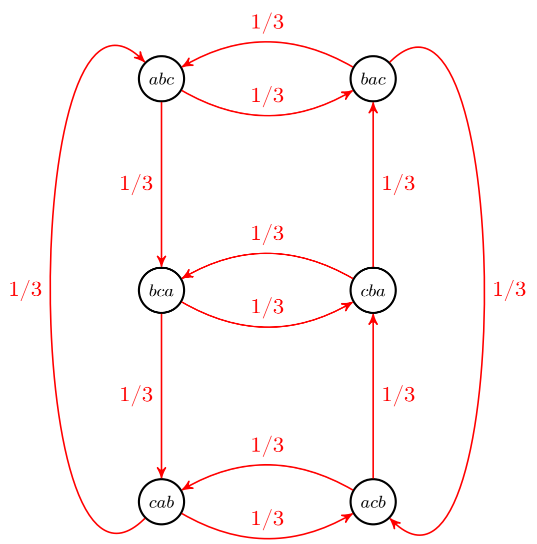
Classroom exercises

5.1 *Card shuffling.* Consider a deck (korttipakka) of $n = 3$ playing cards labeled using a, b, c. The possible configurations of the deck are denoted as $S = \{abc, acb, bac, bca, cab, cba\}$, where in each configuration the cards of the deck are listed from top to bottom. The deck is shuffled as follows: In each step the topmost card is lifted and then pushed to a uniformly random location in the deck, so that the topmost card is placed to the top, middle, or bottom of the deck, each choice with probability $\frac{1}{3}$, and independently of earlier steps. Denote by X_t the configuration of the deck after t shuffling steps.

(a) Explain why (X_t) is a Markov chain, write down its transition matrix, and draw the corresponding transition diagram so that no arrows cross each other.

Solution. (X_t) is a Markov chain because each step is performed independently of earlier steps. The transition matrix (when the states are ordered lexicographically) and the transition diagram (loops excluded) are:

$$P = \begin{bmatrix} \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \end{bmatrix}$$



(b) Find out the invariant distribution π of the chain.

Solution. Because the chain is irreducible (clear from the transition diagram), it has a unique invariant distribution. One can solve manually that the invariant distribution is the uniform distribution on S. One can also note that the matrix

P is special in the sense that, in addition to having unit rows sums (a property of every transition matrix), this matrix has unit column sums. Such matrices are called doubly stochastic, and for such transition matrices the invariant distribution is always uniform.

(c) Is the Markov chain (X_t) reversible with respect to the distribution π?

Solution. No, because for example

$$\pi(abc)P(abc, bca) \;=\; \frac{1}{6}\frac{1}{3} \;\neq\; 0 \;=\; \pi(bca)P(bca, abc).$$

Now consider a deck of 52 cards, labeled as $\{1, 2, \ldots, 52\}$. Let S be the set of all configurations of the deck.

(d) Determine the size of the set S.

Solution. The topmost card can be chosen in 52 ways, and after that the second card in 51 ways, …, and the bottom card in 1 way. Hence by the combinatorial rule of product principle, the number of deck configurations equals

$$|S| \;=\; 52 \cdot 51 \cdot 50 \cdots 2 \cdot 1 \;=\; 52!$$

(e) Describe a Markov chain (X_t) which represents the same shuffling method, at each round lifting the topmost card and placing it to a uniformly random location. How many entries does the corresponding transition matrix have?

Solution. This Markov chain has state space S consisting of all lists of length 52 where each card occurs precisely once. Each such list corresponds to a deck configuration where the cards are listed from top to bottom. Given a deck configuration $x \in S$, denote by $\sigma_k(x)$ the deck configuration obtained by lifting the topmost card in x and replacing it into the deck so that $k-1$ cards are on top of the lifted card. Then the transition matrix of (X_t) can be expressed as

$$P(x,y) \;=\; \begin{cases} \frac{1}{52}, & y = \sigma_k(x) \text{ for some } k = 1, \ldots, 52, \\ 0, & \text{else.} \end{cases}$$

This is a 52!-by-52! square matrix and has $(52!)^2$ entries.

(f) Find out the unique invariant distribution of the Markov chain (X_t) corresponding to the 52-card deck.

Solution. As with the 3-card deck, also the transition matrix corresponding to the 52-card deck is doubly stochastic, and therefore the unique invariant distribution is the uniform distribution on S.

Homework problems

5.2 *Metropolis chain.* Let π be a probability distribution on a finite state space S such that $\pi(x) > 0$ for all $x \in S$. Let Q be an irreducible transition matrix on S. The *Metropolis chain* for π with proposal matrix Q is a Markov chain with transition matrix defined by

$$P(x,y) \;=\; \begin{cases} Q(x,y)A(x,y) & \text{if } y \neq x, \\ 1 - \sum_{z \neq x} Q(x,z)A(x,z) & \text{if } y = x, \end{cases}$$

where $A(x,y) = \min\left(\frac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)}, 1\right)$.

(a) Verify that P really is a transition matrix (has nonnegative entries and unit row sums).

Solution. Because the entries of π and Q are nonnegative, it follows that the offdiagonal entries of P are nonnegative as well. To verify that also the diagonal entries of P are nonnegative, note that because $A(x,y) \leq 1$ and $\sum_z Q(x,z) = 1$,

$$\begin{aligned} P(x,x) \;&=\; 1 - \sum_{z \neq x} Q(x,z)A(x,z) \\ &\geq\; 1 - \sum_{z \neq x} Q(x,z) \;=\; Q(x,x) \;\geq\; 0. \end{aligned}$$

The row sums for each x are

$$\sum_y P(x,y) = \sum_{y \neq x} Q(x,y)A(x,y) + 1 - \sum_{z \neq x} Q(x,z)A(x,z) = 1.$$

We conclude that P is a transition matrix of a Markov chain on S.

(b) Verify that P is reversible with respect to π.

Solution. Note that for any $x \neq y$,

$$\begin{aligned} \pi(x)P(x,y) \;&=\; \pi(x)Q(x,y)A(x,y) \\ &=\; \pi(x)Q(x,y)\min\left(\frac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)},\; 1\right) \\ &=\; \min\left(\pi(x)Q(x,y)\frac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)},\; \pi(x)Q(x,y)\right) \\ &=\; \min\Big(\pi(y)Q(y,x),\; \pi(x)Q(x,y)\Big), \end{aligned}$$

so that we conclude that

$$\pi(x)P(x,y) \;=\; \min\Big(\pi(y)Q(y,x),\; \pi(x)Q(x,y)\Big).$$

Because the right side above is a symmetric function of (x,y), so is the left side, and therefore, $\pi(x)P(x,y) = \pi(y)P(y,x)$. Hence P is reversible with respect to π.

(c) Explain with the help of the ergodic theorem in the lecture notes, how a numerical approximation for a sum $\sum_x \pi(x)f(x)$ can be computed for an arbitrary function f, by simulating a Markov chain having transition matrix P, when we assume that P is irreducible. (Such a method is called Markov chain Monte Carlo simulation.)

Solution. Because P is reversible with respect to π, it follows that

$$\sum_x \pi(x)P(x,y) \;=\; \sum_x \pi(y)P(y,x) \;=\; \pi(y)\sum_x P(y,x) \;=\; \pi(y),$$

so that (as row vector) $\pi = \pi P$, and hence π is an invariant distribution of P. When we assume that P is irreducible, then π is the unique invariant distribution, and by the ergodic theorem,

$$\lim_{t\to\infty} \frac{1}{t}\sum_{s=0}^{t-1} f(X_s) \;=\; \sum_x \pi(x)f(x)$$

with probability one, regardless of the initial state, for a Markov chain (X_t) with transition matrix P. Hence we get an approximation of $\sum_x \pi(x)f(x)$ by starting the chain from an arbitrary state x_0, simulating the Markov chain $X_0, X_1, \dots, X_t$ for a large t with transition probabilities in P, and taking the empirical average of the values $f(X_s)$.

Additional information. Note that P is not always irreducible, even if Q is irreducible. For example in the case where Q is the transition matrix corresponding to a random walk on a directed 3-cycle, P is the identity matrix which is not irreducible. A sufficient condition for P to be irreducible is that Q is irreducible and satisfies $Q(x,y) = 0$ if and only if $Q(y,x) = 0$.

5.3 *Random walk on a graph.* Let G be an undirected graph on the node set $V = \{1, \dots, n\}$ and suppose that the degree $\deg(x)$ of every node x in G is at least 1. A random walk on G proceeds by moving at each step to a neighboring node selected uniformly at random. The random walk is hence a Markov chain with transition matrix given by

$$P(x,y) \;=\; \begin{cases} \frac{1}{\deg(x)}, & \text{if } x \text{ and } y \text{ are neighbors,} \\ 0, & \text{else.} \end{cases}$$

(a) Prove that a random walk on a graph is reversible with respect to the distribution $\pi(x) = c\deg(x)$ when the constant c is chosen appropriately.

Solution. For $\pi(x) = c\deg(x)$ to be a probability distribution, we need to have

$$\sum_x \pi(x) \;=\; 1.$$

This is true when we select $c = (\sum_x \deg(x))^{-1}$. In this case $\pi(x) \ge 0$ for all x, so π is probability distribution. Let us now verify reversibility. (i) If x, y are not neighbors, then

$$\pi(x)P(x,y) \;=\; 0 \;=\; \pi(y)P(y,x).$$

(ii) If x, y are neighbors, then

$$\pi(x)P(x,y) \;=\; c\deg(x)\frac{1}{\deg(x)} \;=\; c \;=\; \pi(y)P(y,x).$$

Hence $\pi(x)P(x,y) = \pi(y)P(y,x)$ for all x, y, so that P is reversible with respect to π.

(b) By using the result of part (a), calculate the invariant distribution for a lone king moving randomly on the standard 8-by-8 chessboard $S = \{\mathtt{a1}, \dots, \mathtt{h8}\}$.

Solution. The king's walk is a random walk of type in (a) on the undirected graph with node set S, where two squares of the chessboard of are neighbors if the king has a feasible move between them. The degrees of the nodes are given by table below.

	a	b	c	d	e	f	g	h
8	3	5	5	5	5	5	5	3
7	5	8	8	8	8	8	8	5
6	5	8	8	8	8	8	8	5
5	5	8	8	8	8	8	8	5
4	5	8	8	8	8	8	8	5
3	5	8	8	8	8	8	8	5
2	5	8	8	8	8	8	8	5
1	3	5	5	5	5	5	5	3

The sum of the degrees equals 420. Hence the unique invariant distribution is given by

$$\pi(x) \;=\; \begin{cases} \frac{3}{420}, & x \text{ is a corner node,} \\ \frac{5}{420}, & x \text{ is a non-corner boundary node,} \\ \frac{8}{420}, & x \text{ is a center node.} \end{cases}$$

(c) By using the result of part (a), calculate the invariant distribution for a lone knight (ratsu) moving randomly on the standard 8-by-8 chessboard $S = \{\mathtt{a1}, \dots, \mathtt{h8}\}$.

Solution. The knight's walk is a similar random walk on a similar graph with node set S. The sum of the degrees equals 336, and the degrees are given by the table below. Hence the unique invariant distribution is obtained by dividing the degrees by 336, similarly as in (b).

	a	b	c	d	e	f	g	h
8	2	3	4	4	4	4	3	2
7	3	4	6	6	6	6	4	3
6	4	6	8	8	8	8	6	4
5	4	6	8	8	8	8	6	4
4	4	6	8	8	8	8	6	4
3	4	6	8	8	8	8	6	4
2	3	4	6	6	6	6	4	3
1	2	3	4	4	4	4	3	2