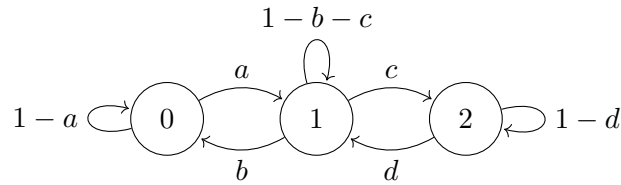


Homework 08

Spring 2024

1. Markov Chain Big Theorem

For this problem we will consider the following three-state chain and illustrate the ideas behind the Markov chain convergence theorem. Here, $a, b, c, d \in (0, 1)$.



- a. Let $T_0 = \min\{n \in \mathbb{Z}_+ : X_n = 0\}$ be the first passage time to state 0. Let $\mu_y := \mathbb{E}_0[\sum_{n=0}^{T_0-1} \mathbb{1}\{X_n = y\}]$ for $y = 0, 1, 2$ be the mean number of visits to state y , starting at 0 and ending right before we return to 0. Explain why $\mu = \mu P$.
- b. Therefore, if we define π to be μ after we normalize it so that the entries sum to 1, π is a stationary distribution. Why is π unique?
- c. Now deduce that $\pi_0 = 1/\mathbb{E}_0[T_0]$. In words, $\mathbb{E}_0[T_0]$ is the mean return time from state 0 to itself.
- d. Explain why the fraction of times $\sum_{m=1}^n \mathbb{1}\{X_m = 0\}$, where n is a positive integer, converges a.s. to π_0 as $n \rightarrow \infty$. (Hint: Define $T_0^{(1)} := T_0$ and for integers $k \geq 2$, define

$$T_0^{(k)} = \min\{n > T_0^{(k-1)} : X_n = 0\} - T_0^{(k-1)}$$

to be the additional time it takes to return to 0 for the k th time. Then $T_0^{(1)}, T_0^{(2)}, T_0^{(3)}, \dots$ are i.i.d. and one can apply the SLLN.)

- e. Consider two copies of the above chain $(X_n, Y_n)_{n \in \mathbb{N}}$, where the chains move independently of each other, Y_0 is picked from the stationary distribution, and X_0 is started from any fixed state x . Explain why the two chains will meet after a finite time, and think about why this implies that the chain started from state x converges in distribution to the stationary distribution π .

Solution:

- a. Here, $\mu_0 = 1$ (since $X_0 = 0$) and $(\mu P)_0 = (1 - a)\mu_0 + b\mu_1 = 1 - a + b\mu_1$. The expected number of visits to state 1, μ_1 , is computed as follows. With probability a , $X_1 = 1$. Conditioned on $X_1 = 1$, the mean number of visits to state 1 before returning to state 0 is $1/b$, since every time we are at state 1 we have a probability b of transitioning to state 0, and so the number of times we stay at state 1 is geometric with parameter b . Plugging in, $(\mu P)_0 = 1 - a + b \cdot a(1/b) = 1$.

Now consider μ_y for $y = 1, 2$. μ_y is the mean number of visits to state y in the period $0, \dots, T_0 - 1$. Meanwhile, $(\mu P)_y = \sum_{x=0,1,2} \mu_x P_{x,y}$, and since μ_x is the mean number of visits to x in times $0, \dots, T_0 - 1$ and $P_{x,y}$ is the probability of transitioning to y , then $\mu_x P_{x,y}$ is the mean number of visits to y in times $1, \dots, T_0$. The insight here is that since we start at state 0 at time 0, and we end at state 0 at time T_0 , the times $0, \dots, T_0 - 1$ and $1, \dots, T_0$ look the same, so the mean number of visits to y is the same for each period. Thus, $\mu = \mu P$.

- b. Uniqueness is harder to justify, but in fact Part (d) below implies that $n^{-1} \sum_{m=1}^n \mathbb{1}\{X_m = y\} \rightarrow 1/\mathbb{E}_y[T_y]$ for all states y as $n \rightarrow \infty$, so by taking expectations of both sides, we obtain $n^{-1} \sum_{m=1}^n \mathbb{P}(X_m = y) \rightarrow 1/\mathbb{E}_y[T_y]$. In particular, if we start the chain from the stationary distribution, then $\mathbb{P}(X_m = y) = \pi(y)$ so $\pi(y) = 1/\mathbb{E}_y[T_y]$, in particular, π is unique.
- c. Note that $\mu_0 + \mu_1 + \mu_2 = \mathbb{E}_0[T_0]$ and $\pi_0 = \mu_0/(\mu_0 + \mu_1 + \mu_2) = 1/\mathbb{E}_0[T_0]$.
- d. Observe that $\sum_{m=1}^{T_0^{(1)} + \dots + T_0^{(k)}} \mathbb{1}\{X_m = 0\} = k$. Thus,

$$\frac{1}{T_0^{(1)} + \dots + T_0^{(k)}} \sum_{m=1}^{T_0^{(1)} + \dots + T_0^{(k)}} \mathbb{1}\{X_m = 0\} = \frac{k}{T_0^{(1)} + \dots + T_0^{(k)}} \rightarrow \frac{1}{\mathbb{E}_0[T_0]}$$

a.s., as $k \rightarrow \infty$, by the SLLN. Also, since $T_0^{(1)} + \dots + T_0^{(k)} \rightarrow \infty$ as $k \rightarrow \infty$, then we also have $n^{-1} \sum_{m=1}^n \mathbb{1}\{X_m = 0\} \rightarrow 1/\mathbb{E}_0[T_0]$ a.s., as $n \rightarrow \infty$. Finally, we use $1/\mathbb{E}_0[T_0] = \pi_0$ from the arguments in the previous parts.

- e. The original chain is aperiodic, which is the condition that we need in order for the product chain $(X_n, Y_n)_{n \in \mathbb{N}}$ to be irreducible (you can convince yourself that if the original chain is periodic, then the product chain is not irreducible). Then, the vector $\tilde{\pi}(x, y) := \pi(x)\pi(y)$ is stationary for the product chain, because the two chains are independent. In particular, $\tilde{\pi}(x, x) = \pi(x)\pi(x) > 0$, so $\mathbb{E}_{(x,x)}[T_{(x,x)}] = 1/\tilde{\pi}(x, x) < \infty$ for any state x , which means that the two chains will meet each other at the state x in finite time.

What is the big deal? In fact $\mathbb{P}(X_n \neq Y_n) \leq \mathbb{P}(T > n)$ for any positive integer n . This is because at time T we can glue the chains together and force them to transition together for the rest of time, so then the event $\{X_n \neq Y_n\}$ exactly becomes the event $\{T > n\}$, i.e., at time n the two chains have not met yet. Now since we have argued that T is finite, $\mathbb{P}(T > n) \rightarrow 0$ as $n \rightarrow \infty$, so $\mathbb{P}(X_n \neq Y_n) \rightarrow 0$ as $n \rightarrow \infty$. However, recall that $(X_n)_{n \in \mathbb{N}}$ is the chain started at x and $(Y_n)_{n \in \mathbb{N}}$ is the stationary chain, so we have argued that the chain started at x is approaching stationarity!

2. Two-State Chain with Linear Algebra

Consider the Markov chain $(X_n, n \in \mathbb{N})$, shown in Figure 1, where $\alpha, \beta \in (0, 1)$.

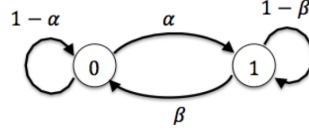


Figure 1: Markov chain for this Problem

- Find the probability transition matrix P .
- Find two real numbers λ_1 and λ_2 such that there exists two non-zero vectors u_1 and u_2 such that $Pu_i = \lambda_i u_i$ for $i = 1, 2$. Further, show that P can be written as $P = U\Lambda U^{-1}$, where U and Λ are 2×2 matrices and Λ is a diagonal matrix.
Hint: This is called the eigendecomposition of a matrix.
- Find P^n in terms of U and Λ for each $n \in \mathbb{N}$.
- Assume that $X_0 = 0$. Use the result in part (c) to compute the PMF of X_n for all $n \in \mathbb{N}$.
- What does the fraction of time spent in state 0, $n^{-1} \sum_{i=1}^n \mathbb{1}\{X_i = 0\}$, converge to (almost surely) as $n \rightarrow \infty$?

Solution:

- The probability transition matrix is

$$P = \begin{bmatrix} 1 - \alpha & \alpha \\ \beta & 1 - \beta \end{bmatrix}.$$

- Since $(P - \lambda_i I)x = 0$ has non-zero solution u_i , we have $\det(P - \lambda_i I) = 0$, i.e., λ_1 and λ_2 are solutions to

$$\det \begin{bmatrix} 1 - \alpha - \lambda & \alpha \\ \beta & 1 - \beta - \lambda \end{bmatrix} = \lambda^2 - (2 - \alpha - \beta)\lambda + 1 - \alpha - \beta.$$

Then we get $\lambda_1 = 1$, and $\lambda_2 = 1 - \alpha - \beta$. Then we can get u_1 and u_2 : $u_1 = [1 \ 1]^\top$ and $u_2 = [\alpha \ -\beta]^\top$. Further, we can see that if we let

$$U = [u_1 \ u_2] = \begin{bmatrix} 1 & \alpha \\ 1 & -\beta \end{bmatrix},$$

and

$$\Lambda = \begin{bmatrix} 1 & 0 \\ 0 & 1 - \alpha - \beta \end{bmatrix},$$

we have $PU = U\Lambda$, which is equivalent to $P = U\Lambda U^{-1}$.

- We have

$$P^n = U\Lambda U^{-1} \dots U\Lambda U^{-1} = U\Lambda^n U^{-1}.$$

d. Let $\pi(n) = [\Pr(X_n = 0) \ \Pr(X_n = 1)]$ be the PMF of X_n . Then we have

$$\pi(n) = \pi(0)P^n = \pi(0)U\Lambda^n U^{-1}.$$

Since we have $\pi(0) = [1 \ 0]$, by some computation, we get

$$\pi(n) = \frac{1}{\alpha + \beta} [\beta + \alpha(1 - \alpha - \beta)^n \ \alpha - \alpha(1 - \alpha - \beta)^n].$$

e. By the Big Theorem, the fraction of time spent in state 0 converges to the stationary distribution at state 0, $\pi(0)$. The stationary distribution is

$$\pi = \frac{1}{\alpha + \beta} [\beta \ \alpha],$$

so $\pi(0) = \beta/(\alpha + \beta)$.

3. Random Walk on an Undirected Graph

Consider a random walk on an undirected connected finite graph (that is, define a Markov chain where the state space is the set of vertices of the graph, and at each time step, transition to a vertex chosen uniformly at random out of the neighborhood of the current vertex). What is the stationary distribution π ? Your answer may depend on $\deg(v)$ (i.e., the degree of a vertex v) for some v . *Hint*: assume first that the chain is *reversible*.

Solution: Let \mathcal{X} be the state space. The stationary distribution is

$$\pi(v) = \frac{\deg(v)}{\sum_{v' \in \mathcal{X}} \deg(v')}, \quad v \in \mathcal{X}.$$

Clearly, π is a valid probability distribution. We check that the chain is reversible. Note that if u and v are neighbors, then

$$\pi(u)P(u, v) = \frac{\deg(u)}{\sum_{v' \in \mathcal{X}} \deg(v')} \cdot \frac{1}{\deg(u)} = \frac{1}{\sum_{v' \in \mathcal{X}} \deg(v')}.$$

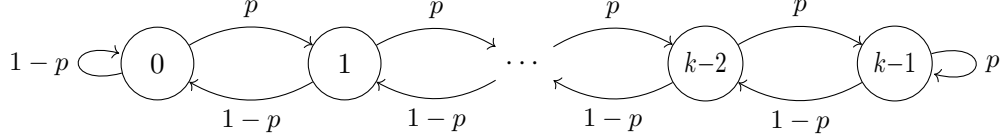
Also,

$$\pi(v)P(v, u) = \frac{\deg(v)}{\sum_{v' \in \mathcal{X}} \deg(v')} \cdot \frac{1}{\deg(v)} = \frac{1}{\sum_{v' \in \mathcal{X}} \deg(v')}.$$

So, $\pi(u)P(u, v) = \pi(v)P(v, u)$ if u and v are neighbors. If u and v are not neighbors, then $P(u, v) = P(v, u) = 0$, so the equation holds in this case as well. The chain is reversible and so π is stationary.

4. Finite Random Walk

Let $0 < p < 1$, and consider the following finite *random walk* with bias p on $\mathcal{X} = \{0, \dots, k-1\}$, also known as the finite *birth-death chain*.



- a. Find the stationary distribution π .

Hint: Write $q = 1 - p$ and define $r := \frac{p}{q}$. Be careful when $r = 1$.

- b. Find the limit of $\pi(0)$ and $\pi(k-1)$, as functions of k , as $k \rightarrow \infty$.

Solution:

- a. Let us solve the detailed balance equations:

$$p \cdot \pi(i-1) = q \cdot \pi(i) \quad \text{for all } i = 1, \dots, k-1,$$

or $\pi(i) = r\pi(i-1)$. Iterating this recurrence relation, we have $\pi(i) = r^i\pi(0)$, so

$$\sum_{i=0}^{k-1} \pi(i) = \pi(0) \sum_{i=0}^{k-1} r^i = \pi(0) \frac{1-r^k}{1-r} = 1.$$

We can then solve for $\pi(0) = \frac{1-r}{1-r^k}$ and $\pi(i) = r^i \frac{1-r}{1-r^k}$ in general. However, this formula is undefined when $r = 1$, or $p = \frac{1}{2}$. Instead, we find that $\pi(i) \equiv \frac{1}{k}$ for all $i = 0, \dots, k-1$. In short, the stationary distribution is given by

$$\pi(i) = \begin{cases} r^i \frac{1-r}{1-r^k} & \text{if } p \neq \frac{1}{2} \\ \frac{1}{k} & \text{if } p = \frac{1}{2}. \end{cases}$$

- b. First, the limit of $\pi(0)$ is $\lim_{k \rightarrow \infty} \frac{1}{k} = 0$ if $r = 1$ and $(1-r) \lim_{k \rightarrow \infty} \frac{1}{1-r^k}$ if $r \neq 1$. Now, $1/(1-r^k) \rightarrow 1$ if $r < 1$ and $\rightarrow 0$ if $r > 1$. Therefore

$$\lim_{k \rightarrow \infty} \pi(0) = \begin{cases} 1-r & \text{if } r < 1 \\ 0 & \text{if } r \geq 1. \end{cases}$$

For $\pi(k-1)$, we know that the limit is also 0 if $r = 1$, so let $r \neq 1$. Then

$$\lim_{k \rightarrow \infty} \pi(k-1) = \lim_{k \rightarrow \infty} \frac{r^{k-1} - r^k}{1 - r^k} = \lim_{k \rightarrow \infty} \frac{1-r}{\frac{1}{r^{k-1}} - r} = \begin{cases} 0 & \text{if } r < 1 \\ \frac{r-1}{r} & \text{if } r > 1. \end{cases}$$

Therefore the limit is

$$\lim_{k \rightarrow \infty} \pi(k-1) = \begin{cases} 0 & \text{if } r \leq 1 \\ 1 - \frac{1}{r} & \text{if } r > 1. \end{cases}$$

5. Metropolis–Hastings

We will prove some properties of the *Metropolis–Hastings* algorithm, an example of Markov Chain Monte Carlo (MCMC) sampling that you will see more of in lab. The goal of MH is to draw samples from a distribution $p(x)$; the algorithm assumes that

- We can compute $p(x)$ up to a normalizing constant C via $f(x)$, and
- We have a proposal distribution $g(x, \cdot)$.

The steps in making a transition are:

- i. Propose the next state y according to the distribution $g(x, \cdot)$.
- ii. Accept the proposal with probability

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

- iii. If the proposal is accepted, move the chain to y ; otherwise, stay at x .

Remark. The normalizing factor $C = 1/\sum_{x \in \mathcal{X}} f(x)$ is sometimes called the *partition function*, and it can be difficult to compute for large sets \mathcal{X} , even if $f(x)$ is efficient to compute.

In the following, we will verify that the Metropolis–Hastings chain has stationary distribution p , and in fact approaches stationarity after running for some time, at which point we can draw samples from p by sampling from the chain.

- a. The key to why Metropolis–Hastings works is the **detailed balance equations**. Suppose we have a finite irreducible Markov chain on a state space \mathcal{X} with transition probability matrix P . Show that if there exists a distribution π on \mathcal{X} satisfying detailed balance,

$$\pi(x)P(x, y) = \pi(y)P(y, x) \quad \text{for all } x, y \in \mathcal{X},$$

then $\pi P = \pi$ is a stationary distribution of the chain.

- b. Returning to the Metropolis–Hastings chain, find $P(x, y)$. For simplicity, assume $x \neq y$.
- c. Show that the target distribution $p(x)$ satisfies the detailed balance equations for $P(x, y)$, and conclude that $p(x)$ is the stationary distribution of the chain.
- d. If the chain is aperiodic, then it will converge to the stationary distribution. If not, we can force the chain to be aperiodic by considering the **lazy chain**: on each transition, the chain decides not to move with probability $\frac{1}{2}$, independently of the propose-accept step. Explain why the lazy chain is aperiodic, and explain why the stationary distribution is the same as before.

Solution:

- a. Suppose that detailed balance holds. Then for all $y \in \mathcal{X}$,

$$(\pi P)(y) = \sum_{x \in \mathcal{X}} \pi(x)P(x, y) = \sum_{x \in \mathcal{X}} \pi(y)P(y, x) = \pi(y) \sum_{x \in \mathcal{X}} P(y, x) = \pi(y).$$

b. $P(x, y)$ is the probability that we propose y with $g(x, \cdot)$, then accept y :

$$P(x, y) = g(x, y)A(x, y) = g(x, y) \min \left\{ 1, \frac{f(y)g(y, x)}{f(x)g(x, y)} \right\}.$$

c. We check that detailed balance holds for any pair of states (x, y) . Observe that if

$$\frac{f(y)g(y, x)}{f(x)g(x, y)} \leq 1,$$

then $A(x, y)$ is equal to this ratio, and its reciprocal is at least 1, which makes $A(y, x) = 1$. Thus, assume without loss of generality that $A(y, x) = 1$, swapping x and y if this were not true. Then $P(y, x) = g(y, x)$, and

$$\begin{aligned} p(x)P(x, y) &= p(x)g(x, y)A(x, y) \\ &= p(x)g(x, y)\frac{f(y)g(y, x)}{f(x)g(x, y)} \\ &= p(x)\frac{f(y)}{f(x)}g(y, x) \\ &= p(y)g(y, x) \\ &= p(y)P(y, x). \end{aligned}$$

Note that $p(x)\frac{f(y)}{f(x)} = p(y)$ follows from the fact that f is directly proportional to p .

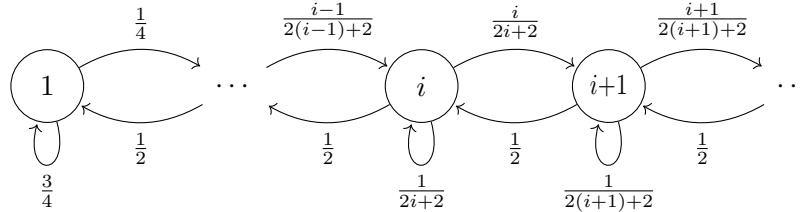
d. The lazy chain is aperiodic as it has self-loops. Now, suppose $\pi = \pi P$ is a stationary distribution of the original chain. The transition probability matrix P' of the lazy chain is $\frac{1}{2}P + \frac{1}{2}I$, where I is the identity matrix, so

$$\pi P' = \frac{1}{2}\pi P + \frac{1}{2}\pi I = \frac{1}{2}\pi + \frac{1}{2}\pi = \pi.$$

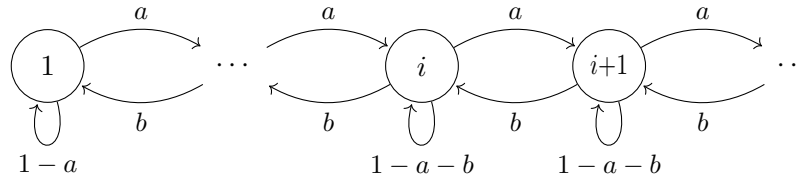
In other words, π is also a stationary distribution for the lazy chain.

6. Markov Chains with Countably Infinite State Space

- a. Show that the Markov chain with state space \mathbb{Z}^+ and the following transition diagram is not positive recurrent. Also find the expected time it takes to return to state i starting from i for any $i \in \mathbb{Z}^+$.



- b. Let $0 < a < b < a + b \leq 1$. Consider now the Markov chain with state space \mathbb{Z}^+ and the following transition diagram:



Show that a stationary distribution of this Markov chain is given by

$$\pi(i) = \left(\frac{a}{b}\right)^{i-1} \left(1 - \frac{a}{b}\right).$$

Also compute the expected time it takes to return to state i starting from i .

Solution:

- a. By the big theorem, an irreducible Markov chain is not positive recurrent if it does not have a stationary distribution. The given chain is a birth-death chain, so any stationary distribution π will satisfy the detailed balance equations, namely

$$\pi(i) \cdot P(i, i+1) = \pi(i+1) \cdot P(i+1, i) \quad \text{for all } i \in \mathbb{Z}^+.$$

With the given transition probabilities, this means

$$\pi(i+1) = \frac{i}{i+1} \pi(i) = \frac{i}{i+1} \frac{i-1}{i} \pi(i-1) = \dots = \frac{1}{i+1} \pi(1).$$

A stationary distribution must also satisfy $\sum_{i=1}^{\infty} \pi(i) = 1$ in order to be a valid probability distribution. However,

$$\sum_{i=1}^{\infty} \pi(i) = \pi(1) \sum_{i=1}^{\infty} \frac{1}{i} = \pi(1) \cdot \infty$$

means that it is impossible to assign a value to $\pi(1)$ such that $\sum_{i=1}^{\infty} \pi(i) = 1$. Therefore this chain does not admit a stationary distribution. The expected return time for any state is ∞ as the chain is not positive recurrent.

b. We first observe that

$$\left(\frac{a}{b}\right)^{i-1} \left(1 - \frac{a}{b}\right) \geq 0,$$
$$\sum_{i=1}^{\infty} \left(\frac{a}{b}\right)^{i-1} \left(1 - \frac{a}{b}\right) = \frac{1}{1 - \frac{a}{b}} \left(1 - \frac{a}{b}\right) = 1,$$

so π is a valid probability distribution. This Markov chain is also a birth-death chain, so we are left to verify that π satisfies the detailed balance equations:

$$\pi(i) \cdot P(i, i+1) = \left(\frac{a}{b}\right)^{i-1} \left(1 - \frac{a}{b}\right) a = \left(\frac{a}{b}\right)^i \left(1 - \frac{a}{b}\right) b = \pi(i+1) \cdot P(i+1, i).$$

In this case, the expected return time is $\frac{1}{\pi(i)} = \left(\frac{b}{a}\right)^{i-1} \frac{b}{b-a}$.

Remark. Part b shows that the stationary distribution of the infinite birth-death chain with bias p is $\text{Geometric}(1 - \frac{p}{q})$. The last line is a rather magical result — once we have the stationary distribution, we immediately know the expected amount of time it takes between successive visits to any given state!