

## Chapter 2

# Markov chain fundamentals

*This chapter introduces Markov chains as a model describing processes that evolve through time, in a sequence of steps. We characterize Markov chains in terms of their long term behavior and discuss how such behavior can be identified in practice. We conclude with an algorithmic application of Markov chains widely used in statistics and optimization.*

### 2.1 Markov chains

Let us start with the following example.

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**Example 2.1**

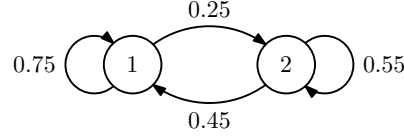
We want to build a model to predict the weather in Lisbon, Portugal. We denote by  $x_0$  the weather today, and by  $x_t$  the weather  $t$  days from today. For simplicity, we consider that each variable  $x_t, t = 0, \dots$ , takes only one of two values: *Sunny* (1) or *Rainy* (2).

After analyzing the statistics of past weeks, we conclude that:

- A sunny day is followed by another sunny day with a probability 0.75, and by a rainy day with probability 0.25.
- A rainy day is followed by another rainy day with a probability 0.55, and by a sunny day with a probability 0.45.

We can represent the above weather dynamics in the form of a *transition diagram*, as depicted in Fig. 2.1. The nodes in the diagram represent the possible values that the variable of interest can take (in this case *Sunny* and *Rainy*), and the edges indicate the probability of a *transition* between the two values in the corresponding direction.

Let us suppose that, today, the weather is *Sunny*, i.e.,  $x_0 = 1$  and we want to determine how likely it is that, two days from today, the weather is *Rainy*. We can use a standard probability reasoning to determine such probability:



**Figure 2.1** Transition diagram representing the weather dynamics in Lisbon, Portugal. Node (1) corresponds to *Sunny* and node (2) corresponds to *Rainy*.

- There is a probability of 0.75 that tomorrow the weather is *Sunny*, i.e.,

$$\mathbb{P}[x_1 = 1 \mid x_0 = 1] = 0.75.$$

In the case that  $x_1 = 1$ , the probability that  $x_2 = 2$  is then 0.25.

- There is a probability of 0.25 that tomorrow the weather is *Rainy*, i.e.,

$$\mathbb{P}[x_1 = 2 \mid x_0 = 1] = 0.25.$$

In the case that  $x_1 = 2$ , the probability that  $x_2 = 2$  is then 0.55.

Then, using the total probability law (see Appendix A, Equation A.34), we get:

$$\begin{aligned} \mathbb{P}[x_2 = 2 \mid x_0 = 1] &= \mathbb{P}[x_2 = 2 \mid x_1 = 1] \mathbb{P}[x_1 = 1 \mid x_0 = 1] + \mathbb{P}[x_2 = 2 \mid x_1 = 2] \mathbb{P}[x_1 = 2 \mid x_0 = 1] \\ &= 0.25 \times 0.75 + 0.55 \times 0.25 = 0.325. \end{aligned}$$

We can also represent the transition probabilities as a *matrix*:

$$\mathbf{P} = \begin{bmatrix} 0.75 & 0.25 \\ 0.45 & 0.55 \end{bmatrix},$$

where

$$[\mathbf{P}]_{i,j} = \mathbb{P}[x_{t+1} = j \mid x_t = i], \quad i, j \in \{1, 2\}.$$

Using this representation, and letting  $\boldsymbol{\mu}_t$  denote a *row vector* such that

$$\mu_{t,i} = \mathbb{P}[x_t = i], \quad i \in \{1, 2\},$$

we can write the fact that today is *Sunny* as

$$\boldsymbol{\mu}_0 = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

and the weather for tomorrow can be computed directly as

$$\mu_1 = \mu_0 \mathbf{P} = \begin{bmatrix} 0.75 & 0.25 \end{bmatrix}.$$

Finally, we can replicate the computation above to obtain the weather prediction two days from today:

$$\mu_2 = \mu_1 \mathbf{P} = \begin{bmatrix} 0.675 & 0.325 \end{bmatrix}.$$

In Example 2.1 we build a probabilistic model to describe/predict the temporal evolution of some entity of interest—in this case, the weather. Later on, we use a similar approach to describe the interaction between a decision-maker and the environment. We represent the information to be monitored at each time step  $t$  as a r.v.  $x_t$ , and refer to the sequence  $\{x_t, t \in \mathbb{N}\}$  as a *stochastic process*. The r.v.  $x_t$  is called the *state of the process at time  $t$* , and we refer to the set of possible values of  $x_t$  the *state space of the process*, denoted as  $\mathcal{X}$ .

In the model of Example 2.1, the weather at day  $t$  can be predicted directly from the weather at day  $t - 1$ . Such property—whereby the state of the process at step  $t$  depends only on the state of the process at step  $t - 1$ —is present in many processes of interest and is known as the *Markov property*.

### Markov property

A stochastic process  $\{x_t, t \in \mathbb{N}\}$  with state space  $\mathcal{X}$  has the *Markov property* if, for any time step  $t \in \mathbb{N}$ ,

$$\mathbb{P}[x_t = y \mid \mathbf{x}_{0:t-1} = \mathbf{x}_{0:t-1}] = \mathbb{P}[x_t = y \mid x_{t-1} = x_{t-1}]. \quad (2.1)$$

A stochastic process verifying the Markov property is called a *Markov chain*.

The Markov property implies that Markov chains are *memoryless*: the history of the process plays no role in determining its future evolution (except for the present state). It also implies that the dynamics of a Markov chain are completely described by the corresponding *transition probabilities*. Moreover, in many practical problems, the dependence of the transition probabilities on  $t$  can be safely disregarded. This means that, for every pair  $(x, y) \in \mathcal{X} \times \mathcal{X}$ , there is a value  $P_{x,y}$  such that, for all  $t \in \mathbb{N}$ ,

$$P_{x,y} = \mathbb{P}[x_t = y \mid x_{t-1} = x]. \quad (2.2)$$

When that is the case, the Markov chain is called *time-homogeneous*. Except where explicitly noted, Markov chains throughout the book are assumed time-homogeneous.

As seen in Example 2.1, given a (time-homogeneous) Markov chain, the transition probabilities  $P_{x,y}$  in (2.2) can be collected in a *transition probability matrix*

$\mathbf{P}$ , with

$$[\mathbf{P}]_{x,y} = P_{x,y} \stackrel{\text{def}}{=} \mathbb{P}[x_t = y \mid x_{t-1} = x],$$

with  $x, y \in \mathcal{X}$ . Conversely, if  $\mathbf{P}$  is a  $N \times N$  stochastic matrix,<sup>1</sup> then we can define a Markov chain over  $\mathcal{X} = \{1, \dots, N\}$  with transition probability matrix  $\mathbf{P}$ . At this point, it should be clear that any (time-homogeneous) Markov chain is completely described by:

- Its state space,  $\mathcal{X}$ ;
- Its transition probabilities,  $\mathbf{P}$ ;
- Its initial state,  $x_0$ .

When the initial state is not known beforehand, we may instead specify an *initial distribution*  $\mu_0$  for  $x_0$ . In light of the above, we henceforth refer to a Markov chain either as a sequence  $\{x_t, t \in \mathbb{N}\}$  or, more commonly, as a tuple  $\mathcal{M} = (\mathcal{X}, \mathbf{P}, \mu_0)$ . Whenever the initial distribution is immaterial for our discussion, we instead adopt the more compact representation  $\mathcal{M} = (\mathcal{X}, \mathbf{P})$ .

We conclude with two notational remarks. First, it will often be convenient to emphasize the nature of  $\mathbf{P}$  as a conditional probability. For this reason, we write  $\mathbf{P}(y \mid x)$  to denote the  $(x, y)$  element of matrix  $\mathbf{P}$ . Second, if  $\mu$  is a distribution over the state space  $\mathcal{X}$  of a Markov chain, it will sometimes be convenient to represent such distribution as a row vector  $\boldsymbol{\mu}$ , as was done in Example 2.1. We use  $\mu(x)$  and  $\mu_x$  interchangeably with the same meaning.

### 2.1.1 Skeleton chains and the Chapman-Kolmogorov equation

As seen in Example 2.1, the transition probabilities allow for long-term predictions about the state of the chain. Let  $\mathcal{M} = (\mathcal{X}, \mathbf{P}, \mu_0)$  denote a Markov chain, and suppose that we want to make a prediction regarding the state of the chain at time step  $t = 1$ . Then, using the total probability law,

$$\mathbb{P}[x_1 = y] = \sum_{x \in \mathcal{X}} \mathbb{P}[x_1 = y \mid x_0 = x] \mathbb{P}[x_0 = x]. \quad (2.3)$$

All probabilities on the right-hand side of (2.3) can be expressed directly in terms of the Markov chain model components, yielding

$$\begin{aligned} \mathbb{P}[x_1 = y] &= \sum_{x \in \mathcal{X}} \mathbf{P}(y \mid x) \mu_0(x) \\ &= [\boldsymbol{\mu}_0 \mathbf{P}]_y. \end{aligned}$$

Let  $\mu_1$  denote the resulting probability distribution, i.e.,

$$\mu_1(x) = \mathbb{P}[x_1 = x].$$

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<sup>1</sup>A *stochastic matrix* is a square matrix with non-negative entries where each row adds to 1.

Repeating the process for time step  $t = 2$ , we get

$$\begin{aligned}\mathbb{P}[x_2 = y] &= \sum_{x \in \mathcal{X}} \mathbb{P}[x_2 = y \mid x_1 = x] \mathbb{P}[x_1 = x] \\ &= \sum_{x \in \mathcal{X}} \mathbf{P}(y \mid x) \mu_1(x) \\ &= \boldsymbol{\mu}_1 \mathbf{P} = \boldsymbol{\mu}_0 \mathbf{P}^2.\end{aligned}$$

More generally, we have that

$$\mathbb{P}[x_t = y] = \boldsymbol{\mu}_0 \mathbf{P}^t. \quad (2.4)$$

On the other hand, we can express  $\mathbb{P}[x_t = y]$  in terms of the initial distribution  $\mu_0$  using the total probability law to get

$$\mathbb{P}[x_t = y] = \sum_{x \in \mathcal{X}} \mathbb{P}[x_t = y \mid x_0 = x] \mathbb{P}[x_0 = x]. \quad (2.5)$$

Equating (2.4) and (2.5), we immediately get that

$$[\mathbf{P}^t]_{x,y} = \mathbb{P}[x_t = y \mid x_0 = x],$$

and we refer to  $\mathbf{P}^t$  as the *t-step transition probability matrix*. Since  $\mathbf{P}^t$  is a stochastic matrix, we can use it to define a new Markov chain  $\mathcal{M}' = (\mathcal{X}, \mathbf{P}^t, \mu_0)$ . The chain  $\mathcal{M}'$  describes the evolution of the original chain  $\mathcal{M}$  every  $t$  steps, and is known as the *t-skeleton for the chain  $\mathcal{M}$* . As with  $\mathbf{P}$ , we write  $\mathbf{P}^t(y \mid x)$  to denote the  $(x, y)$  element of  $\mathbf{P}^t$ , to emphasize the nature of  $\mathbf{P}^t$  as a conditional (transition) probability.

### Chapman-Kolmogorov equation

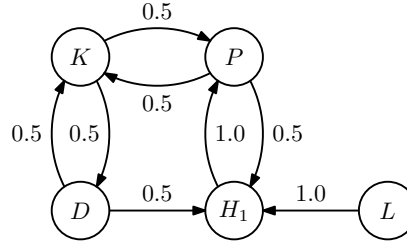
We just saw that, given a Markov chain  $(\mathcal{X}, \mathbf{P}, \mu_0)$ , the state of the chain at any time step  $t_1$  can be characterized by the distribution

$$\mu_{t_1}(y) = \mathbb{P}[x_{t_1} = y] = [\boldsymbol{\mu}_0 \mathbf{P}^{t_1}]_y.$$

We can, in turn, use  $\mu_{t_1}$  to compute the distribution of the state at some posterior time step  $t_1 + t_2$  as

$$\mu_{t_1+t_2}(y) = [\boldsymbol{\mu}_{t_1} \mathbf{P}^{t_2}]_y.$$

Bringing the two together, we obtain the *Chapman-Kolmogorov equation* for Markov chains, which translates the simple matrix fact that  $\mathbf{P}^{t_1+t_2} = \mathbf{P}^{t_1} \mathbf{P}^{t_2}$ .



**Figure 2.2** Transition diagram representing the motion of the robot in monitoring mode.

### Chapman-Kolmogorov equation

Given a Markov chain  $\{x_t, t \in \mathbb{N}\}$  with state space  $\mathcal{X}$ ,

$$\mathbb{P}[x_{t_1+t_2} = y \mid x_0 = x] = \sum_{z \in \mathcal{X}} \mathbb{P}[x_{t_1} = z \mid x_0 = x] \mathbb{P}[x_{t_1+t_2} = y \mid x_{t_1} = z].$$

## 2.1.2 Examples

We encountered a first example of a Markov chain in Example 2.1. We now complement that first example with a number of additional examples in different domains of application. Some of these examples rely on technicalities that are specific to the corresponding area of application and are, for that reason, only glossed over. The purpose is not to dwell on the specificities of the example, but rather on the overall principles guiding the modeling process.

### Household robot

Consider the domestic robot scenario described in Section 1.1. In it, a mobile robot moves around a household environment, assisting the human inhabitants in their domestic chores.

Suppose that the robot is set to “monitoring mode”: it departs from the Living room and repeatedly visits the “public areas” of the house (Kitchen, Pantry, Dining room and Hallway 1), monitoring environment variables in these areas. For simplicity, we assume that the transitions between areas always succeed. However, upon reaching an area, the robot randomly selects which area to visit next.

The motion of the robot can be described as a Markov chain, corresponding to the transition diagram of Fig. 2.2. The state of the chain at each time step  $t$  is just the position of the robot at that time step; it provides all information necessary to predict the future evolution of the chain.

Formally, representing the Markov chain as a triplet  $(\mathcal{X}, \mathbf{P}, x_0)$ , we have that

- The state space is  $\mathcal{X} = \{L, K, P, D, H_1\}$ ;
- The transition probability matrix is

$$P = \begin{array}{ccccc} \begin{bmatrix} 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 0.0 \\ 0.0 & 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \end{bmatrix} & \begin{matrix} L \\ K \\ P \\ D \\ H_1 \end{matrix} \\ \begin{matrix} L & K & P & D & H_1 \end{matrix} & \end{array}$$

where we marked in gray the states corresponding to each row and column.

- $x_0 = L$ .

Using the Markov chain model, we can predict the position of the robot at different time steps, using fact that  $x_0 = L$ . For mathematical convenience, we express the fact that  $x_0 = L$  as

$$\mu_0 = [1 \ 0 \ 0 \ 0 \ 0],$$

which then yields

$$\mu_1 = \mu_0 P = [0 \ 0 \ 0 \ 0 \ 1].$$

As expected, after departing from the Living room, the robot will end in the Hallway with probability 1. Continuing the computation, we get

$$\begin{aligned} \mu_2 &= \mu_1 P = \mu_0 P^2 = [0 \ 0 \ 1 \ 0 \ 0] \\ \mu_3 &= \mu_2 P = \mu_0 P^3 = [0 \ 0.5 \ 0 \ 0 \ 0.5] \\ \mu_4 &= \mu_3 P = \mu_0 P^4 = [0 \ 0 \ 0.75 \ 0.25 \ 0] \\ \mu_5 &= \mu_4 P = \mu_0 P^5 = [0 \ 0.5 \ 0 \ 0 \ 0.5], \end{aligned}$$

after which the predictions enter cycle, alternating between

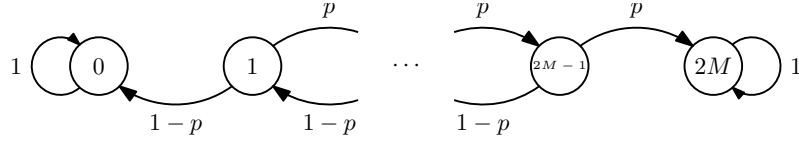
$$\mu_{\text{even}} = [0 \ 0 \ 0.75 \ 0.25 \ 0]$$

and

$$\mu_{\text{odd}} = [0 \ 0.5 \ 0 \ 0 \ 0.5].$$

### Player's ruin

Consider the situation of a gambler, Adam, entering a casino with  $M$  euros. Adam decides to play a game of chance (e.g., the roulette) that proceeds as follows. At each round of the game, he bets 1 euro; there is a probability  $p$  of winning, in which case Adam receives the 1 euro back plus 1 additional euro. If Adam loses, on the other hand, he loses his bet. Adam will quit either when his money runs out or when he doubles the amount of money he started with. We assume that consecutive games are independent of one another.



**Figure 2.3** Transition diagram representing the evolution of Adam's fortune.

In this case, we want to predict the money that Adam will make or lose in the game. Since consecutive games are independent, the only information that we need to predict Adam's fortune after a game is Adam's fortune before the game. For this reason, Adam's fortune evolves according to a Markov chain  $(\mathcal{X}, \mathbf{P}, M)$ , where

- The state space is  $\mathcal{X} = \{0, \dots, 2M\}$ ;
- The transition probability between any two states  $x, y \in \mathcal{X}$  is given by

$$P(y | x) = \begin{cases} 1 & \text{if } x = y = 0 \text{ or } x = y = 2M \\ p & \text{if } 0 < x < 2M \text{ and } y = x + 1 \\ 1 - p & \text{if } 0 < x < 2M \text{ and } y = x - 1 \\ 0 & \text{otherwise.} \end{cases}$$

- $x_0 = M$ .

We can also represent the Markov chain using the transition diagram in Fig. 2.3.

To illustrate the evolution of the chain, we show in Fig. 2.4 the average fortune of the gambler's fortune as time goes by. In the plot of Fig. 2.4 we consider  $M = 5$  and show the average evolution of the chain  $\{x_t\}$  for different values of  $p$ .

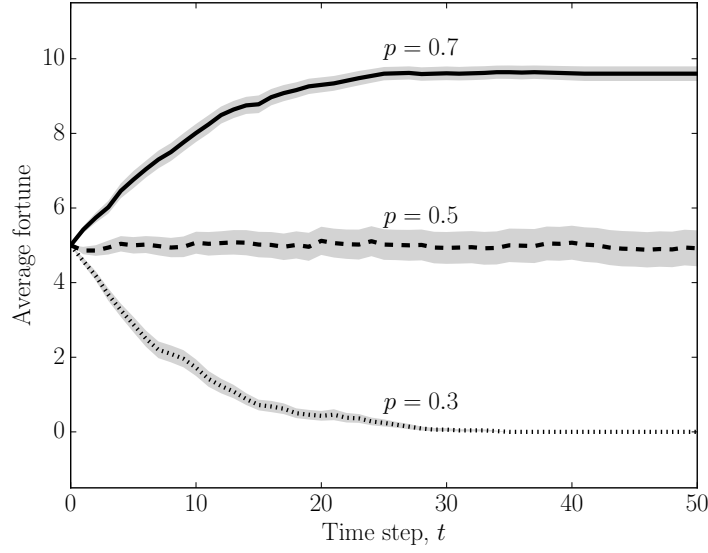
### Supermarket queue

We now describe the time evolution of the number of customers in a supermarket queue. We assume that the cashier is able to dispatch, in average, a customer every  $1/\mu$  time units, for some  $\mu > 0$ . Conversely, a new customer joins the queue every  $1/\lambda$  time units, for some  $\lambda > 0$  and such that  $\lambda < \mu$ . In other words, the *arrival rate*,  $\lambda$ , is smaller than the *service rate*,  $\mu$ , for otherwise the size of the queue would keep increasing.

Since, at each moment, the number of customers in the queue depends only on the number of customers in the queue in the moment immediately before and the service and arrival rates, we can model the number of customers in the queue using a Markov chain. We consider the state of the chain at time step  $t$ ,  $x_t$ , to be the number of customers in the queue after  $t$  time units have elapsed.

Two observations are in order: first, the state space of the chain consists of all non-negative integers. Unlike the chains considered thus far, the state space is, therefore, infinite. Second, under certain technical conditions that we do not detail here, it can then be shown that





**Figure 2.4** Evolution of the Adam's fortune for different values of  $p$ . If  $p > \frac{1}{2}$ , Adam eventually doubles his fortune. Conversely, if  $p < \frac{1}{2}$ , Adam eventually goes bankrupt. Finally, if  $p = \frac{1}{2}$ , Adam's fortune remains approximately constant.

- The probability of 0 arrivals and 0 departures in a unit of time is approximately given by

$$p_{00} \approx 1 - (\lambda + \mu);$$

- The probability of 0 arrivals and 1 departure is approximately given by

$$p_{01} \approx \mu;$$

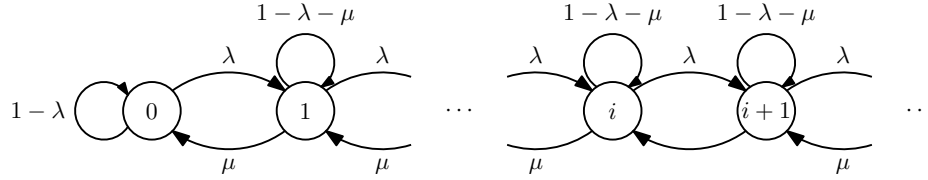
- The probability of 1 arrival and 0 departures is approximately given by

$$p_{10} \approx \lambda.$$

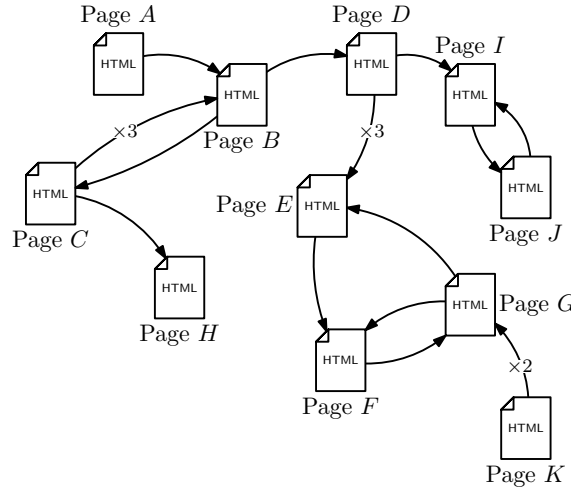
Taking the above information into account, we finally get:

$$\begin{aligned} P(0 | 0) &\approx 1 - \lambda; \\ P(i | i) &\approx 1 - \lambda - \mu, & \text{for } i > 0; \\ P(i + 1 | i) &\approx \lambda; \\ P(i - 1 | i) &\approx \mu, & \text{for } i > 0; \\ P(j | i) &\approx 0, & \text{for } j \notin \{i, i + 1, i - 1\}; \end{aligned}$$

The Markov chain thus obtained is represented in the transition diagram depicted in Fig. 2.5.



**Figure 2.5** Transition diagram for the supermarked queue.

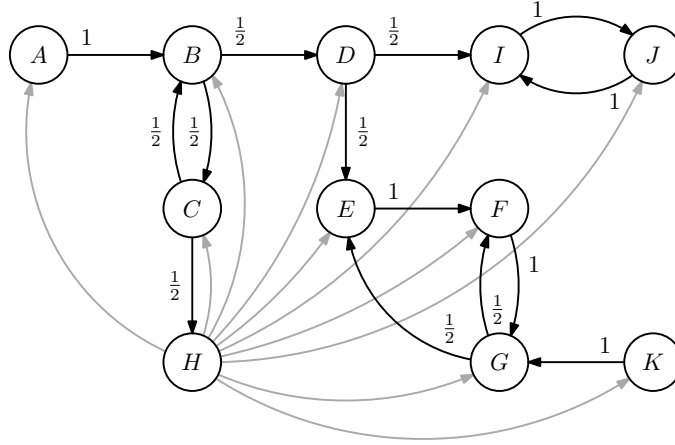


**Figure 2.6** Graph depicting a set of mutually referencing web pages. An edge from page  $a$  to page  $b$  labeled with “ $\times k$ ” indicates that page  $a$  includes  $k$  references to page  $b$ , where labels “ $\times 1$ ” have been omitted.

### The PageRank algorithm

PAGERANK is the algorithm developed by Google for their web search engine to order the results of a particular search. Conceptually, PAGERANK simulates a “random crawler” navigating through the retrieved set of documents/webpages. At each time step, the crawler visits one of the pages; with uniform probability, the crawler selects one of the pages referenced in the current page and moves to that page. The rank of a page thus translates the amount of time that the crawler spends in that specific page.

To illustrate the steps of the algorithm, let us consider the set of pages depicted in Fig. 2.6, where we included an arrow from page  $a$  to page  $b$  whenever  $a$  includes a reference to  $b$ . The topology of the resulting “network of documents” is similar to the topology of the transition diagram describing the movement of the random crawler: each document corresponds to a node in the graph, and a vertex between two nodes  $a$  and  $b$  is added whenever  $a$  refers  $b$  (multiple references are ignored). Additionally, to handle pages with no references (such as  $H$  in Fig. 2.6), PAGERANK artificially adds references from such pages to all other pages. The resulting Markov chain is represented in the transition diagram of Fig. 2.7, where



**Figure 2.7** Transition diagram for the Markov chain corresponding to the set of mutually referencing web pages in Fig. 2.7. Gray edges correspond to the artificially added references.

- The state space is  $\mathcal{X} = \{A, B, C, D, E, F, G, H, I, J, K\}$ ;
- Denoting by  $\text{succ}(a)$  the set of states corresponding to pages referred in  $a$ , the transition probability between any two states  $x, y \in \mathcal{X}$  is given by

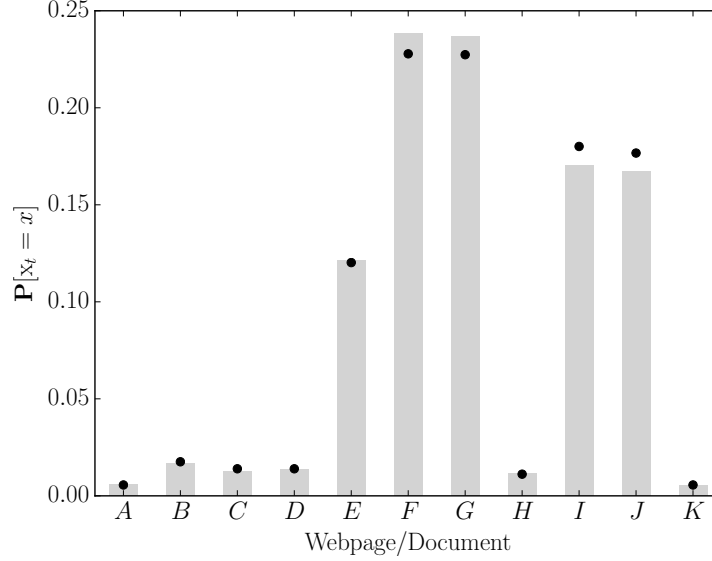
$$P(y | x) = \begin{cases} \frac{1}{|\text{succ}(x)|} & \text{if } y \in \text{succ}(x); \\ 0 & \text{otherwise.} \end{cases} \quad (2.6)$$

PAGERANK includes an additional artifact to avoid being trapped in a subset of pages that only refer to one another (such as pages  $I$  and  $J$  in Fig. 2.6). Sets of self-referencing pages may be quite large and, therefore, hard to detect. For this reason, at every time step the crawler “teleports” to one randomly selected page with probability  $1 - \gamma$ , for some positive  $\gamma < 1$ .

To determine the rank of a page  $a$ , we analyze the “amount of time” that, in the long run, the crawler spends in page  $a$  in comparison with the other pages. The analysis of such long-term behavior is the focus of Section 2.2, where we establish how such analysis can be performed. For now, it suffices to say that the amount of time that the chain spends in an arbitrary state  $x$  is captured by the probability  $\mathbb{P}[x_t = x]$ , for sufficiently large  $t$ . We assume that such probability becomes “stable” for  $t$  sufficiently large, i.e., large  $t$ ,

$$\mathbb{P}[x_t = x] = \mathbb{P}[x_{t-1} = x] = \mu(x) \quad (2.7)$$

for large  $t$ .



**Figure 2.8** Comparison between the analytical solution of (2.9) (circles) and the empirical distribution obtained by simulating a crawler navigating the pages in Fig. 2.6 according to the PAGERANK algorithm (bars).

Bringing the teleportation probability into play in (2.7), we get

$$\begin{aligned} \mathbb{P}[x_t = x] &= \sum_{y \in \mathcal{X}} \mathbb{P}[x_t = x \mid x_{t-1} = y] \mathbb{P}[x_{t-1} = y] \\ &= \frac{1-\gamma}{|\mathcal{X}|} + \gamma \sum_{y \in \mathcal{X}} P(x \mid y) \mathbb{P}[x_{t-1} = y], \end{aligned}$$

where  $\mathbf{P}$  is as defined in (2.6). This finally yields the linear system of equations

$$\boldsymbol{\mu} = \frac{1-\gamma}{|\mathcal{X}|} \mathbf{1} + \gamma \boldsymbol{\mu} \mathbf{P}. \quad (2.8)$$

We can solve (2.8) for  $\boldsymbol{\mu}$  to get

$$\boldsymbol{\mu} = \frac{1-\gamma}{|\mathcal{X}|} \mathbf{1}^\top (\mathbf{I} - \gamma \mathbf{P}^\top)^{-1}, \quad (2.9)$$

where  $\mathbf{I}$  is the identity matrix and  $\mathbf{1}$  is the all-ones (column) vector. We compare in Fig. 2.8 the rank computed analytically using (2.9) and the values obtained by running an actual crawler in the “web” of Fig. 2.6.

## 2.2 Stability of Markov chains

This section categorizes Markov chains in terms of their long-term behavior, formalizing some of the ideas explored in the PAGERANK example. To that purpose,

we start by classifying the states of a Markov chain according to three criteria, assessing

- Whether a state can be visited by the chain;
- Whether such visits occur in a cyclic pattern;
- Whether such visits are frequent.

Together, these three classification criteria provide the means to assess if, in the long run, a given Markov chain exhibits stable behavior, in a sense soon to be made clear.

### 2.2.1 Classification of Markov chain states

This subsection discusses *accessibility*, *periodicity* and *recurrence* of states, and how such properties allow us to make statements regarding the behavior of the Markov chain as a whole.

#### Irreducibility

We first consider the ability of a Markov chain to reach different parts of its state space. Given a Markov chain  $(\mathcal{X}, \mathbf{P})$ , a state  $y \in \mathcal{X}$  is *accessible* from state  $x \in \mathcal{X}$  or, equivalently, that *state  $x$  leads to state  $y$* , if the chain can reach state  $y$  from state  $x$ . Formally,  $x$  leads to  $y$  if

$$\mathbb{P}[x_t = y \mid x_0 = x] > 0 \quad (2.10)$$

for some  $t \in \mathbb{N}$  or, in terms of the transition probability matrix, if

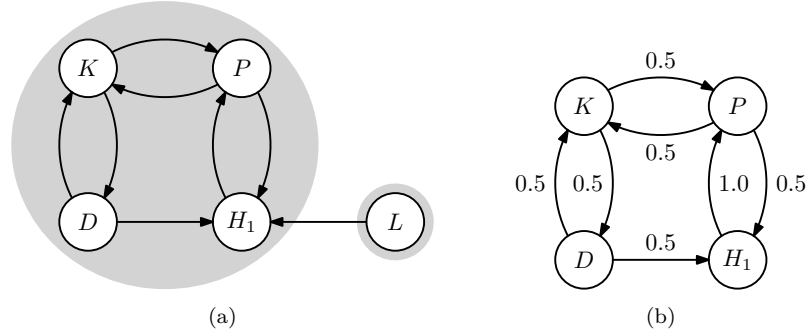
$$\mathbf{P}^t(y \mid x) > 0$$

for some  $t \in \mathbb{N}$ . We write  $x \rightarrow y$  to indicate that  $x$  leads to  $y$ ,  $x, y \in \mathcal{X}$ . Two states  $x, y \in \mathcal{X}$  *communicate* if  $x \rightarrow y$  and  $y \rightarrow x$ . We write  $x \leftrightarrow y$  to indicate that  $x$  and  $y$  are communicating states.

#### Irreducible Markov chain

A Markov chain  $(\mathcal{X}, \mathbf{P})$  is *irreducible* if, for any states  $x, y \in \mathcal{X}$ ,  $x \leftrightarrow y$ , and *reducible* otherwise.

The relation “ $\leftrightarrow$ ” is an *equivalence relation* (see Exercise 2.1). Therefore, we can partition the state space of a Markov chain into *communicating classes*; an irreducible Markov chain has a single communicating class, while reducible Markov chains have multiple classes.



**Figure 2.9** (a) Communicating classes in the household robot example from page 16. (b) Reduced Markov chain for the household robot example. In this reduced chain, there is a single communicating class, so the chain is irreducible.

### Example 2.2

Let us analyze the weather example from page 11. Any of the two states can be reached from the other state, meaning that there is a single communicating class, corresponding to the whole state space,  $\mathcal{X}$ .

### Example 2.3

Analyzing the household robot example from page 16, we note that the state space  $\mathcal{X}$  can be partitioned in two communicating classes,  $\mathcal{X}_0 = \{L\}$  and  $\mathcal{X}_1 = \{K, P, D, H_1\}$ , as outlined in Fig. 2.9(a). Thus, the chain is reducible. We can, however, redefine the Markov chain to consider only the states in  $\mathcal{X}_1$ . Such reduced chain is represented in the transition diagram of Fig. 2.9(b) and is now irreducible. The transition probabilities for this chain are similar to those of the original chain, except that the row and column corresponding to state  $L$  are removed:

$$P = \begin{bmatrix} 0.0 & 0.5 & 0.5 & 0.0 \\ 0.5 & 0.0 & 0.0 & 0.5 \\ 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 1.0 & 0.0 & 0.0 \end{bmatrix}.$$

Irreducibility thus indicates whether a chain cannot be reduced to a smaller chain, as we just did.

### Aperiodicity

A second aspect to consider when analyzing a Markov chain is whether or not it exhibits *cyclic behavior*. Given a Markov chain  $(\mathcal{X}, P)$ , the *period of a state*  $x \in \mathcal{X}$ , denoted as  $d_x$ , is the *greatest common divider* of all steps at which state  $x$  can be

visited, i.e.,

$$d_x = \gcd \{t \in \mathbb{N} \mid \mathbf{P}^t(x \mid x) > 0, t > 0\}.$$

Intuitively, if a state  $x \in \mathcal{X}$  has period  $d_x$ , then the number of steps between two consecutive visits to  $x$  is always a multiple of  $d_x$ . A state  $x \in \mathcal{X}$  with  $d_x = 1$  is called *aperiodic*. Otherwise, it is called *periodic with period  $d_x$* .

### Aperiodic Markov chain

A Markov chain  $(\mathcal{X}, \mathbf{P})$  is *aperiodic* if all states  $x \in \mathcal{X}$  are aperiodic, and *periodic* otherwise.

#### Example 2.4

We again analyze the weather example from page 11. Since, in this case,  $\mathbf{P}(x \mid x) > 0$  for all  $x \in \mathcal{X}$ , the period of both states is 1 and the chain is aperiodic.

#### Example 2.5

Let us consider the reduced version of the household robot example in Fig. 2.9(b). As seen before, it is represented as an irreducible Markov chain  $(\mathcal{X}, \mathbf{P})$ , with  $\mathcal{X} = \{K, P, D, H_1\}$  and

$$\mathbf{P} = \begin{bmatrix} 0.0 & 0.5 & 0.5 & 0.0 \\ 0.5 & 0.0 & 0.0 & 0.5 \\ 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 1.0 & 0.0 & 0.0 \end{bmatrix}.$$

To compute the period of each state  $x \in \mathcal{X}$ , we look at the different powers of  $\mathbf{P}$  and observe the elements in the main diagonal, corresponding to the probabilities  $\mathbf{P}^t(x \mid x)$ . We have that

$$\mathbf{P}^2 = \begin{bmatrix} 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.75 & 0.25 & 0.0 \\ 0.0 & 0.75 & 0.25 & 0.0 \\ 0.5 & 0.0 & 0.0 & 0.5 \end{bmatrix}, \quad \mathbf{P}^3 = \begin{bmatrix} 0.0 & 0.75 & 0.25 & 0.0 \\ 0.5 & 0.0 & 0.0 & 0.5 \\ 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.75 & 0.25 & 0.0 \end{bmatrix},$$

and  $\mathbf{P}^4 = \mathbf{P}^2$ . Therefore, for each state  $x \in \mathcal{X}$ , we have that

$$\{t \in \mathbb{N} \mid \mathbf{P}^t(x \mid x) > 0, t > 0\} = \{2, 4, 6, 8, \dots\}$$

and  $d_x = 2$ . The chain is, therefore, periodic with period  $d = 2$ .

Aperiodic chains exhibit several properties of interest for the analysis of their long-term behavior. First of all, if  $(\mathcal{X}, \mathbf{P})$  is aperiodic, then there is  $T < \infty$  such that  $\mathbf{P}^t(x | x) > 0$  for all  $t > T$  and all  $x \in \mathcal{X}$  (see Exercise 2.2).

A second important property follows from the fact that, given any two states  $x, y \in \mathcal{X}$  such that  $x \leftrightarrow y$ ,  $d_x = d_y$  (see Exercise 2.3). As such, if  $\mathcal{M} = (\mathcal{X}, \mathbf{P})$  is an irreducible chain and there is  $x \in \mathcal{X}$  such that  $x$  is aperiodic, then  $\mathcal{M}$  is aperiodic. More generally, all states in an irreducible chain have the same period  $d$ , and we refer to  $d$  as the *period of the chain*.

One final property that follows from the two above is that, if  $(\mathcal{X}, \mathbf{P})$  is aperiodic and irreducible, then there is  $T < \infty$  such that  $\mathbf{P}^t(y | x) > 0$  for all  $t > T$  and all  $x, y \in \mathcal{X}$ .

### Recurrence

A third and final aspect that we look at is how often a chain visits a state and how long a chain spends in that state. As we discuss in the continuation, the two concepts are essentially equivalent in terms of what they tell us about the behavior of the chain.

Given a Markov chain  $(\mathcal{X}, \mathbf{P})$  and a state  $x \in \mathcal{X}$ , we denote by  $T_x$  the r.v. corresponding to the first time step (after  $t = 0$ ) that the chain visits  $x$  and by  $\eta_x$  the r.v. corresponding to the number of visits (after  $t = 0$ ) to  $x$ . Formally,

$$T_x = \min \{t \in \mathbb{N} \mid x_t = x, t > 0\}$$

$$\eta_x = \sum_{t=1}^{\infty} \mathbb{I}[x_t = x]$$

where, as seen in Chapter 1,  $\mathbb{I}[A]$  denotes the indicator function for the event  $A$ .  $T_x$  and  $\eta_x$  are usually known as the *first return time to  $x$*  and the *occupation time of  $x$* , respectively.

Recurrence is a property of those states that are visited an infinite number of times by the chain. Formally, a state  $x \in \mathcal{X}$  is *recurrent* if  $\mathbb{E}[\eta_x] = \infty$  or, equivalently, if  $\mathbb{P}[T_x < \infty \mid x_0 = x] = 1$ . In contrast, a state  $x \in \mathcal{X}$  is *transient* if  $\mathbb{E}[\eta_x] < \infty$  or, equivalently, if  $\mathbb{P}[T_x < \infty \mid x_0 = x] < 1$ .

#### Recurrent and transient Markov chain

A Markov chain is *recurrent* if all its states are recurrent. It is *transient* if all its states are transient.

If a state  $x \in \mathcal{X}$  is recurrent and  $x \rightarrow y$ , with  $y \in \mathcal{X}$ , then  $y$  is also recurrent and, furthermore,  $y \rightarrow x$ . This implies that an irreducible Markov chain is either transient or recurrent.



### 2.2.2 Stationary and limiting distributions

We now move to the analysis of the long term behavior of Markov chains. In particular, the end goal of this subsection is to introduce a powerful result allowing us to identify Markov chains that eventually settle in what we call *stationary distributions*.

Given a Markov chain  $(\mathcal{X}, \mathbf{P})$ , a distribution  $\mu$  over  $\mathcal{X}$  is a *stationary distribution* for the chain if, for any  $x \in \mathcal{X}$ ,

$$\mu(x) = (\mu \mathbf{P})(x) \stackrel{\text{def}}{=} \sum_{y \in \mathcal{X}} \mu(y) \mathbf{P}(x | y). \quad (2.11)$$

Writing (2.11) in vector notation yields

$$\mu = \mu \mathbf{P},$$

showing that a stationary distribution  $\mu$  is a left eigenvector of the transition probability matrix  $\mathbf{P}$  associated with an eigenvalue of 1. Additionally, if  $\mu$  is a stationary distribution for the chain  $(\mathcal{X}, \mathbf{P})$ , it is also a stationary distribution for any  $t$ -skeleton  $(\mathcal{X}, \mathbf{P}^t)$ .

#### Positive and null chain

A Markov chain  $(\mathcal{X}, \mathbf{P})$  is a *positive chain* if it possesses a stationary probability distribution. It is a *null chain* otherwise.

Stationary distributions are the central concept in the analysis of long-term behavior of Markov chains. In fact, given a Markov chain  $(\mathcal{X}, \mathbf{P}, \mu_0)$ , if the chain eventually settles in some limit distribution  $\lim_{t \rightarrow \infty} \mu_0 \mathbf{P}^t$ , then such distribution must be stationary. To see why, let  $\hat{\mu} = \lim_{t \rightarrow \infty} \mu_0 \mathbf{P}^t$ , assuming that such limit exists. Then,

$$\hat{\mu} = \lim_{t \rightarrow \infty} \mu_0 \mathbf{P}^t = \lim_{t \rightarrow \infty} \mu_0 \mathbf{P}^{t+1} = \lim_{t \rightarrow \infty} \mu_0 \mathbf{P}^t \mathbf{P} = \hat{\mu} \mathbf{P}. \quad (2.12)$$

In the remainder of this section, we establish two fundamental results. First, given a Markov chain  $\mathcal{M} = (\mathcal{X}, \mathbf{P})$ , we identify a set of conditions on  $\mathcal{M}$  that guarantee that a stationary distribution exists for  $\mathcal{M}$ . In particular, we show that if  $\mathcal{M}$  is both *irreducible* and *aperiodic*, then  $\mathcal{M}$  has a stationary distribution,  $\mu^*$ .

Second, given a positive Markov chain, we show that the stationary distribution is unique and  $\mu_0 \mathbf{P}^t \rightarrow \mu^*$ , for any initial distribution  $\mu_0$ . Such convergence result, known as *Markov chain ergodic theorem*, is the key result of this chapter. However, proving both results involves some work that can safely be skipped in a first reading.

**Existence of a stationary distribution** (★)

We establish the following key result.

**Theorem 2.1.** *Let  $\mathcal{M} = (\mathcal{X}, P)$  denote an irreducible and aperiodic Markov chain. Then,  $\mathcal{M}$  possesses a stationary distribution.*

Theorem 2.1 is established in a constructive manner: we identify a “candidate” mapping  $\mu^* : \mathcal{X} \rightarrow \mathbb{R}$  and show that it verifies all required properties of a stationary distribution.

◇

Consider an arbitrary state  $x^* \in \mathcal{X}$  and let  $\eta_{x|x^*}$  denote the expected number of visits to state  $x$  between two visits to state  $x^*$ ,  $x \in \mathcal{X}$ . Formally,

$$\eta_{x|x^*} = \sum_{t=0}^{\infty} \mathbb{P}[x_t = x, t < T_{x^*} \mid x_0 = x^*].$$

Define the mapping  $\mu^* : \mathcal{X} \rightarrow \mathbb{R}$  as

$$\mu^*(x) = \frac{\eta_{x|x^*}}{\mathbb{E}[T_{x^*} \mid x_0 = x^*]},$$

for  $x \in \mathcal{X}$ . The value  $\mu^*(x)$  corresponds to the ratio of time that the chain spends in  $x$  between two visits to the reference state  $x^*$ . The next result ensures that  $\mu^*$  is well defined.

**Lemma 2.2.** *Let  $(\mathcal{X}, P)$  denote an irreducible and aperiodic Markov chain. Then, for any  $x, y \in \mathcal{X}$ ,*

$$\mathbb{P}[T_y < \infty \mid x_0 = x] = 1$$

and

$$\mathbb{E}[T_y \mid x_0 = x] < \infty.$$

*Proof.* See Section 2.6. □

From Lemma 2.2 and definition of  $\eta_{x|x^*}$ , it follows that  $0 \leq \mu^*(x) < \infty$ . To see that  $\mu^*$  is stationary note that, for  $x \neq x^*$ ,

$$\begin{aligned} \eta_{x|x^*} &= \sum_{t=0}^{\infty} \mathbb{P}[x_t = x, T_{x^*} > t \mid x_0 = x^*] \\ &= \sum_{t=1}^{\infty} \mathbb{P}[x_t = x, T_{x^*} > t - 1 \mid x_0 = x^*], \end{aligned}$$

where the above equalities follow from the fact that  $x \neq x^*$ . Then,

$$\begin{aligned}
 \eta_{x|x^*} &= \sum_{t=1}^{\infty} \sum_{y \in \mathcal{X}} \mathbb{P}[x_t = x, T_{x^*} > t-1 \mid x_{t-1} = y, x_0 = x^*] \\
 &\quad \cdot \mathbb{P}[x_{t-1} = y, T_{x^*} > t-1 \mid x_0 = x^*] \\
 &= \sum_{t=1}^{\infty} \sum_{y \in \mathcal{X}} P(x \mid y) \mathbb{P}[x_{t-1} = y, T_{x^*} > t-1 \mid x_0 = x^*] \\
 &= \sum_{y \in \mathcal{X}} P(x \mid y) \sum_{t=1}^{\infty} \mathbb{P}[x_{t-1} = y, T_{x^*} > t-1 \mid x_0 = x^*] \\
 &= \sum_{y \in \mathcal{X}} P(x \mid y) \eta_{y|x^*}.
 \end{aligned}$$

On the other hand,

$$\begin{aligned}
 \eta_{x^*|x^*} &= 1 \\
 &= \sum_{t=1}^{\infty} \mathbb{P}[T_{x^*} = t \mid x_0 = x^*] \\
 &= \sum_{t=1}^{\infty} \sum_{y \in \mathcal{X}} \mathbb{P}[x_{t-1} = y, T_{x^*} = t \mid x_0 = x^*] \\
 &= \sum_{t=1}^{\infty} \sum_{y \in \mathcal{X}} \mathbb{P}[x_{t-1} = y, T_{x^*} > t-1 \mid x_0 = x^*] P(x^* \mid y) \\
 &= \sum_{y \in \mathcal{X}} P(x^* \mid y) \sum_{t=1}^{\infty} \mathbb{P}[x_{t-1} = y, T_{x^*} > t-1 \mid x_0 = x^*] \\
 &= \sum_{y \in \mathcal{X}} P(x^* \mid y) \eta_{y|x^*}.
 \end{aligned}$$

It follows that

$$\mu^*(x) = \sum_{y \in \mathcal{X}} P(x^* \mid y) \mu^*(y), \quad \text{for all } x \in \mathcal{X}.$$

To see that  $\mu^*$  is a distribution, we note that

$$\begin{aligned}
 \mathbb{E}[T_{x^*} \mid x_0 = x^*] &= \sum_{t=0}^{\infty} \mathbb{P}[T_{x^*} > t \mid x_0 = x^*] \\
 &= \sum_{t=0}^{\infty} \sum_{x \in \mathcal{X}} \mathbb{P}[x_t = x, T_{x^*} > t \mid x_0 = x^*] \\
 &= \sum_{x \in \mathcal{X}} \sum_{t=0}^{\infty} \mathbb{P}[x_t = x, T_{x^*} > t \mid x_0 = x^*] = \sum_{x \in \mathcal{X}} \eta_{x|x^*}.
 \end{aligned}$$

With this, all statements in Theorem 2.3 are established.

**Markov chain ergodic theorem** (★)

We now establish the main result of this chapter.

**Theorem 2.3.** *Let  $(\mathcal{X}, \mathbf{P}, \mu_0)$  denote an irreducible and aperiodic Markov chain, with arbitrary initial distribution  $\mu_0$ . Then, if  $\mu^*$  is the corresponding stationary distribution,*

$$\lim_{t \rightarrow \infty} d(\mu_0 \mathbf{P}^t, \mu^*) = 0, \quad (2.13)$$

where  $d(p, q)$  denotes the total variation distance<sup>2</sup> between distributions  $p$  and  $q$ .

The importance of Theorem 2.3 stems from the fact that long-term predictions regarding the chain become independent of the initial distribution and the transition probabilities. In a sense, the chain converges to an *equilibrium distribution*, which has many useful applications in simulation and optimization. We review one of the best known applications in the next section.

◇

To establish the desired result, let  $\mu^*$  denote the stationary distribution for a irreducible and aperiodic Markov chain  $\{x_t, t \in \mathbb{N}\}$ . We compactly denote such chain as  $\mathcal{M} = (\mathcal{X}, \mathbf{P}, \mu_0)$ , where  $\mu_0$  is an arbitrary initial distribution. Similarly, let  $\mathcal{M}'$  refer to a second Markov chain,  $\{y_t, t \in \mathbb{N}\}$ , where now  $\mathcal{M}' = (\mathcal{X}, \mathbf{P}, \mu^*)$ . Note that  $\mathcal{M}$  and  $\mathcal{M}'$  are two independent replicas of the same underlying Markov chain, differing only on their initial distribution.

Let  $T_M$  denote the first time-step at which the two chains meet, i.e.,

$$T_M = \min \{t \in \mathbb{N} \mid x_t = y_t, t > 0\},$$

where  $x_t$  and  $y_t$  denote the states of  $\mathcal{M}$  and  $\mathcal{M}'$  at time step  $t$ , respectively. The desired result follows from the fact that the two chains will surely meet, i.e.,

**Lemma 2.4.** *With probability 1,  $T_M < \infty$ .*

*Proof.* See Section 2.6. □

We now construct a process  $\{z_t, t \in \mathbb{N}\}$  as follows. For  $t \leq T_M$ ,  $z_t = x_t$ . For  $t \geq T_M$ ,  $z_t = y_t$ . By construction,  $\{z_t\}$  is a time-homogeneous Markov chain with state space  $\mathcal{X}$  and transition probabilities  $\mathbf{P}$ .<sup>3</sup> Additionally,  $\mathbb{P}[z_0 = x] = \mu_0(x)$ ,

<sup>2</sup>See Appendix A.

<sup>3</sup>Even if the “state-generating process” for  $\{z_t, t \in \mathbb{N}\}$  is different before and after  $t = T_M$ , both processes verify the Markov property and have the same transition probabilities.

which implies that

$$\mu_t(x) \stackrel{\text{def}}{=} \mathbb{P}[Z_t = x] = [\mu_0 \mathbf{P}^t]_x.$$

Finally, we get that

$$\begin{aligned} \mu_t(x) - \mu^*(x) &= \mathbb{P}[Z_t = x] - \mathbb{P}[Y_t = x] \\ &\leq \mathbb{P}[Z_t = x, Y_t \neq x] \\ &\leq \mathbb{P}[Z_t \neq Y_t] = \mathbb{P}[T_M > t]. \end{aligned}$$

and

$$\mu^*(x) - \mu_t(x) = \mathbb{P}[Y_t = x] - \mathbb{P}[Z_t = x] \leq \mathbb{P}[Y_t = x, Z_t \neq x] \leq \mathbb{P}[T_M > t].$$

Thus,

$$|\mu^*(x) - \mu_t(x)| \leq \mathbb{P}[T_M > t]$$

for all  $x \in \mathcal{X}$ , and the statement of Theorem 2.3 follows directly from Lemma 2.4.

◇

Theorem 2.3 establishes that an irreducible aperiodic Markov chain  $(\mathcal{X}, \mathbf{P})$  converge to its stationary distribution,  $\mu^*$ . A positive Markov chain that converges to its stationary distribution is known as *ergodic*; Theorem 2.3 is, therefore, known as the *ergodic theorem for Markov chains*.

Theorem 2.3 can be further strengthened, by noting that, for any  $t, T > 0$ ,

$$d(\mu^*, \mu_t) \leq K \mathbb{P}[T_M > kT]$$

with  $k = \lfloor t/T \rfloor$ . Moreover, for  $T$  sufficiently large (see Section 2.6),

$$\mathbb{P}[T_M > kT] \leq (1 - p^2)^k.$$

Putting everything together, we can conclude that there is a constant  $0 < \rho < 1$  such that

$$d(\mu^*, \mu_t) \leq K \rho^k,$$

which implies that the convergence of the chain to  $\mu^*$  takes place at a geometric rate. Such a chain is designated *geometrically ergodic*. Moreover, it follows directly from Theorem 2.3 that the stationary distribution of an irreducible and aperiodic Markov chain is unique (see Exercise 2.4).

## 2.3 Markov chains with general state spaces (★)

The treatment of Markov chains with general state spaces requires significantly more involved machinery. However, much of the concepts and results carry almost unchanged from the discrete case. The added effort in the study of general state space chains lies precisely in bringing out structure that makes this class of processes similar to its discrete/finite counterpart.

This section provides a brief overview of some of the main concepts and results in the theory of general state space Markov chains. The goal is not to go into the technical details—for which we refer to the excellent monograph of Meyn and Tweedie (2009). Instead, we seek to emphasize the close relation with the theory for discrete chains discussed in the previous sections.

◇

Consider a stochastic process  $\{x_t, t \in \mathbb{N}\}$ , where each random variable  $x_t$  takes values in a general set  $\mathcal{X}$ , and let  $\sigma(\mathcal{X})$  denote a countably generated  $\sigma$ -algebra on  $\mathcal{X}$ . For simplicity, we assume that all relevant probability measures can be expressed in terms of densities w.r.t. some underlying measure on  $\sigma(\mathcal{X})$ .

As before, the process  $\{x_t, t \in \mathbb{N}\}$  is a Markov chain if it verifies the *Markov property*, i.e., if

$$\mathbb{P}[x_{t+1} \in U \mid \mathbf{x}_{0:t-1} = \mathbf{x}_{0:t-1}] = \mathbb{P}[x_{t+1} \in U \mid x_t = x_{t-1}]$$

for any set  $U \in \sigma(\mathcal{X})$ . We again focus on *time-homogeneous Markov chains*, i.e., chains in which the transition probabilities are independent of  $t$ . When that is the case, the transition probabilities can be collected in a *transition probability kernel*  $\mathbf{P}$  such that

$$\int_U \mathbf{P}(y \mid x) dy = \mathbb{P}[x_{t+1} \in U \mid x_t = x].$$

A Markov chain is thus fully specified as a triplet  $(\mathcal{X}, \mathbf{P}, \mu_0)$  where  $\mu_0$  is the *initial distribution* for the chain, and verifies

$$\mathbb{P}[x_0 \in U] = \int_U \mu_0(x) dx.$$

with  $U \in \sigma(\mathcal{X})$ . For simplicity of notation, given a distribution  $\mu$  over  $\mathcal{X}$ , we often write  $\mu(U)$  and  $\mathbf{P}(U \mid x)$  to denote

$$\mu(U) \stackrel{\text{def}}{=} \int_U \mu(x) dx \quad \text{and} \quad \mathbf{P}(U \mid x) \stackrel{\text{def}}{=} \int_U \mathbf{P}(y \mid x) dy.$$

Additionally, the notion of  $t$ -skeleton remains unchanged, with the  $t$ -step transition probability defined recursively as

$$\mathbf{P}^t(U \mid x) \stackrel{\text{def}}{=} \mathbb{P}[x_t \in U \mid x_0 = x] = \int_{\mathcal{X}} \mathbf{P}(U \mid y) \mathbf{P}^{t-1}(y \mid x) dy,$$

with  $\mathbf{P}^1 = \mathbf{P}$ .

### 2.3.1 Stability concepts in Markov chains with general state space

The main concepts regarding the stability of Markov chains with general state space closely mirror those already introduced for discrete/finite chains. The technical challenge is translating concepts that were introduced for single states to general spaces, where the probability of isolated states is, in general, zero.

*Small sets* play, in the theory of general Markov chains, the role that single states play in discrete Markov chains. Formally, a set  $C \in \mathcal{X}$  is a  $\mu_t$ -small set (or just small set), for  $t > 0$ , if there is  $\varepsilon > 0$  and a function  $\mu_t : \mathcal{X} \rightarrow \mathbb{R}$  such that  $\mu(x) \geq 0$  for all  $x \in \mathcal{X}$  and, for any set  $U \in \sigma(\mathcal{X})$  and any  $x \in C$ ,

$$\mathbf{P}^t(U \mid x) \stackrel{\text{def}}{=} \mathbb{P}[\mathbf{x}_t \in U \mid \mathbf{x}_0 = x] \geq \varepsilon \int_U \mu(x) dx.$$

Intuitively, states in  $C$  behave as a whole, since the ( $t$ -step) transition probabilities out of  $C$  can be made “approximately independent” of the specific state  $x \in C$ . Armed with the notion of small set, it is now possible to generalize the notions of irreducibility, aperiodicity and recurrence to chains with general state space.

### $\psi$ -irreducibility

In the discrete case, an irreducible chain is such that any state can eventually be reached with positive probability from any other state. In the theory of Markov chains with general state space, the corresponding concept is  $\psi$ -irreducibility. A Markov chain is  $\psi$ -irreducible if any sufficiently large set can eventually be reached with positive probability from any state.

#### $\varphi$ -irreducibility

Given a Markov chain  $\mathcal{M} = (\mathcal{X}, \mathbf{P})$  and a non-trivial distribution  $\varphi$  on  $\sigma(\mathcal{X})$ , the chain  $\mathcal{M}$  is  $\varphi$ -irreducible if, for any state  $x \in \mathcal{X}$  and any set  $U \in \sigma(\mathcal{X})$ , there is  $t > 0$  such that

$$\mathbf{P}^t(U \mid x) > 0$$

whenever  $\varphi(U) > 0$ .

It can be shown that if  $(\mathcal{X}, \mathbf{P})$  is  $\varphi$ -irreducible chain for some distribution  $\varphi$ , then it is also  $\psi$ -irreducible, where  $\psi$  is a *maximal irreducibility distribution*, i.e., a distribution over  $\mathcal{X}$  such that

- $\psi(U) \geq \varphi(U)$  for all  $U \in \sigma(\mathcal{X})$ ;
- If  $\psi(U) = 0$  for some  $U \in \sigma(\mathcal{X})$ , then the set of states  $x$  for which

$$\sum_{t=0}^{\infty} \mathbf{P}^t(U \mid x) > 0$$

has null  $\psi$ -probability.

Henceforth, whenever we refer to a  $\psi$ -irreducible chain, it is implicit that  $\psi$  is a maximal irreducibility measure.<sup>4</sup>

<sup>4</sup>Given a  $\psi$ -irreducible Markov chain, any two maximal irreducibility measures are equivalent.

### Aperiodicity

In the theory of general state space Markov chains, small sets act as the counterparts to individual states in the theory of discrete Markov chains. Hence, periodicity is defined in terms of the existence of cyclic patterns in the visits to small sets.

Let us then suppose that a Markov chain  $\mathcal{M} = (\mathcal{X}, \mathbf{P})$  has a set  $C \in \sigma(\mathcal{X})$  that is a  $\mu_T$ -small, for some  $T > 0$ , and such that  $\int_C \mu_T(x) dx > 0$  (i.e., there is a positive probability of the chain returning to  $C$  after  $T$  steps). Let

$$d = \gcd \{t > 0 \mid C \text{ is } \mu_t\text{-small, for some } \mu_t = k_t \mu_T, \text{ with } k_t > 0\}. \quad (2.14)$$

Intuitively, the set in (2.14) includes all time steps in which there is a positive probability of the chain returning to  $C$ . When such a set  $C$  exists, we say that the chain has a *cycle of length*  $d$ .

An important property of  $\psi$ -irreducible chains is that its state space can be partitioned in a family  $\mathcal{D} = \{D_1, \dots, D_d\}$  of disjoint sets such that  $\mathbf{P}(D_{k+1} \mid x) = 1$  for every  $x \in D_k$ ,  $k = 1, \dots, d \pmod{d}$ . The family  $\mathcal{D}$  is called a *d-cycle*, and the largest  $d$  for which there is a *d-cycle* is called the *period* of  $\mathcal{M}$ .

#### Aperiodic Markov chain

A  $\psi$ -irreducible Markov chain  $(\mathcal{X}, \mathbf{P})$  is *aperiodic* if it has period  $d = 1$ , and *periodic* otherwise.

### Recurrence and transience

As in the discrete case, given a Markov chain  $(\mathcal{X}, \mathbf{P})$  and a set  $U \in \sigma(\mathcal{X})$ , we denote by  $\eta_U$  and  $T_U$  the *occupation time* of  $U$  and the *return time to*  $U$ , respectively. Formally,

$$\eta_U = \sum_{t=1}^{\infty} \mathbb{I}[x_t \in U];$$

$$T_U = \min \{t \in \mathbb{N} \mid x_t \in U, t > 0\}.$$

A set  $U$  is called *recurrent* if  $\mathbb{E}[\eta_U \mid x_0 = x] = \infty$  for all  $x \in \mathcal{X}$  and *transient* otherwise. In particular, if there is  $M > 0$  such that  $\mathbb{E}[\eta_U \mid x_0 = x] \leq M$  for all  $x \in \mathcal{X}$ , the set  $U$  is called *uniformly transient*.



**Recurrent and transient Markov chain**

A  $\psi$ -irreducible Markov chain is *recurrent* if every set  $U \in \sigma(\mathcal{X})$  such that  $\psi(U) > 0$  is recurrent. Otherwise, the chain is *transient* and there is a countable family of sets,  $\mathcal{D} = \{D_1, D_2, \dots\}$ , where each  $D_k \in \mathcal{D}$  is transient and

$$\bigcup_{D_k \in \mathcal{D}} D_k = \mathcal{X}.$$

Thus, recurrence means that all “large” subsets of  $\mathcal{X}$  are visited an infinite number of times in expectation. However, it is possible to further strengthen the notion of recurrence—namely, when all “large” sets are visited an infinite number of times *with probability 1*. A set  $U \in \sigma(\mathcal{X})$  is *Harris recurrent* if, for any  $x \in \mathcal{X}$ ,

$$\mathbb{P}[\eta_U = \infty] = 1.$$

A  $\psi$ -irreducible Markov chain is Harris recurrent if every set  $U \in \sigma(\mathcal{X})$  such that  $\psi(U) > 0$  is Harris recurrent. Note that, in the discrete case, Harris recurrence and recurrence coincide.

**2.3.2 Stationary distributions and ergodicity**

The notion of stationary distribution extends trivially to Markov chains with general state spaces. Given a Markov chain  $(\mathcal{X}, \mathbf{P})$ , a function  $\mu^* : \mathcal{X} \rightarrow \mathbb{R}$  is an *invariant* for the chain if  $\mu^*(x) > 0$  for all  $x \in \mathcal{X}$  and, given any set  $U \in \sigma(\mathcal{X})$ ,

$$\int_U \mu^*(x) dx = \int_{\mathcal{X}} \mathbf{P}(U \mid x) \mu^*(x) dx.$$

If, additionally,

$$\int_{\mathcal{X}} \mu^*(x) dx = 1,$$

then  $\mu^*$  is a *stationary distribution for the chain*.

**Positive and null chain**

A  $\psi$ -irreducible Markov chain is a *positive chain* if it possesses a stationary probability distribution. It is a *null chain* otherwise.

Establishing existence of, uniqueness of or convergence to stationary distributions is significantly more involved in Markov chains with general state spaces, and falls outside the scope of this book. In any case, and for completeness, we include without proof three key results that

- Identify conditions under which an invariant is guaranteed to exist;
- Identify conditions under which a chain is positive, i.e., a stationary distribution is guaranteed to exist;
- Identify conditions under which a chain is ergodic, i.e., the chain converges to the stationary distribution.

We refer to the book of Meyn and Tweedie (2009) for a detailed treatment of Markov chains. The first result identifies conditions for the existence of an invariant.

**Theorem 2.5.** *Let  $\mathcal{M} = (\mathcal{X}, P)$  denote a recurrent chain. Then  $\mathcal{M}$  possesses a unique (up to constant multiples) invariant  $\mu^*$ .*

The next result identifies conditions for positivity of a chain.

**Theorem 2.6.** *Let  $\mathcal{M} = (\mathcal{X}, P)$  denote a  $\psi$ -irreducible recurrent chain with invariant  $\mu$ . Then, if there is a small set  $C \in \sigma(\mathcal{X})$  such that  $\psi(C) > 0$  and*

$$\mathbb{E}[T_C \mid x_0 = x] < \infty$$

*for all  $x \in \mathcal{X}$ , the chain is positive Harris recurrent. In particular, it possesses a stationary distribution.*

Together, the two results above extend Theorem 2.1 to general Markov chains. We conclude with a generalization of Theorem 2.3.

**Theorem 2.7.** *Let  $(\mathcal{X}, P)$  be a  $\psi$ -irreducible, aperiodic, positive Harris chain with stationary distribution  $\mu^*$ . Then, for any initial distribution  $\mu_0$  on  $\sigma(\mathcal{X})$ ,*

$$\lim_{t \rightarrow \infty} d(\mu_0 P^t, \mu^*) = 0.$$

### 2.3.3 Example

As an example of a Markov chain with general state space, let us consider the linear system described by difference equation

$$x_{t+1} = ax_t + w_{t+1}, \tag{2.15}$$

where each  $x_t$  and  $w_t$  take values in  $\mathbb{R}$  and each  $w_t$  is a noise term with known distribution that is independent of  $\{x_0, \dots, x_{t-1}\}$  and  $\{w_0, \dots, w_{t-1}\}$ . This model

is known in the literature as an *autoregressive model of order 1*, or AR(1). It is the simplest of a collection of models used in the analysis of time-series.

In virtue of our independence assumptions, the process  $\mathcal{M} = \{x_t, t \in \mathbb{N}\}$  is a Markov chain. For concreteness, let us assume that  $a < 1$  and each  $w_t$  follows a distribution  $\text{Normal}(0, 1)$ . We now analyze the stability of the chain  $\mathcal{M}$ .

In order for  $\mathcal{M}$  to be  $\psi$ -irreducible, we must identify an irreducibility distribution  $\varphi$  such that, for every measurable set  $U \subset \mathbb{R}$  and every state  $x$ ,

$$\sum_{t=0}^{\infty} P^t(U \mid x) > 0$$

whenever  $\varphi(U) > 0$ . For any initial state  $x \in \mathcal{X}$ ,

$$x_t = a^t x + \sum_{\tau=1}^t a^{t-\tau} w_{\tau},$$

which implies that  $x_t$  is a sum of normally distributed r.v.s and, therefore, is also normally distributed, with

$$\begin{aligned} \bar{x}_t &= \mathbb{E}[x_t \mid x_0 = x] = a^t x \\ s_t^2 &= \text{var}[x_t] = \sum_{\tau=1}^t a^{2(t-\tau)} = \sum_{\tau=0}^{t-1} a^{2\tau}. \end{aligned} \tag{2.16}$$

But then,

$$P^t(y \mid x) = \frac{1}{\sqrt{2\pi s_t^2}} \exp \left[ -\frac{(y - \bar{x}_t)^2}{2s_t^2} \right]$$

and is, therefore,  $\psi$ -irreducible. Additionally, it follows from the definition that the chain is also aperiodic.

Taking the limit of (2.16) as  $t \rightarrow \infty$ , since  $a < 1$ , we get

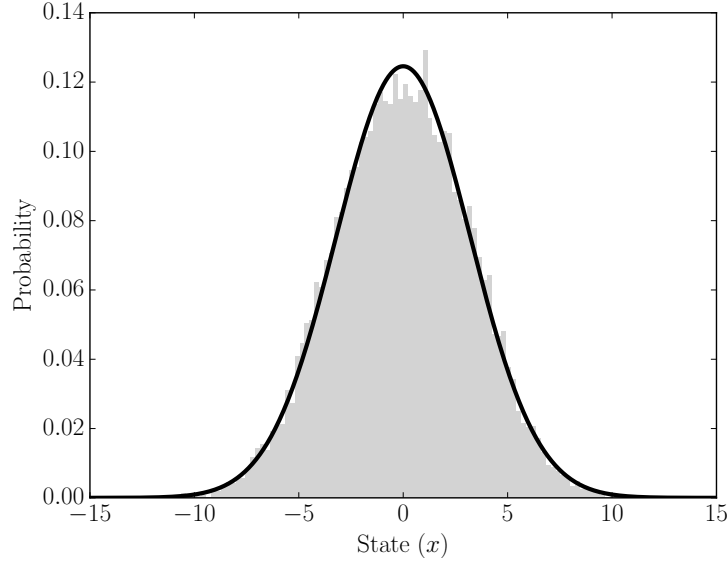
$$\bar{x}_{\infty} = 0 \qquad s_{\infty}^2 = \frac{1}{1-a^2},$$

and the  $\text{Normal}(0, 1/(1-a^2))$  as a candidate for stationary distribution. Suppose then that

$rvarx_t$  is distributed according to  $\text{Normal}(0, 1/(1-a^2))$ . The r.v.  $x_{t+1}$ , being the sum of two normally distributed r.v.s ( $x_t$  and  $w_t$ ) is also normally distributed with

$$\bar{x}_{t+1} = a \cdot 0 + 0 = 0 \qquad s_{t+1}^2 = \frac{a^2}{1-a^2} + 1 = \frac{1}{1-a^2},$$

and we showed that, indeed, the chain is positive and, as a consequence of Theorem 2.7, ergodic. Figure 2.10 depicts the theoretical distribution (solid line) and the empirical distribution (gray bars), obtained by sampling the trajectories of an actual chain.



**Figure 2.10** Theoretical (solid line) and empirical (gray bars) stationary distributions for the linear model in (2.15) with  $a = 0.95$ .

## 2.4 Markov chain Monte Carlo (★)

We conclude this chapter by providing an overview of a class of methods known globally as *Markov chain Monte Carlo* (MCMC). To motivate the need for this class of methods, let us suppose that we wish to determine

$$f = \mathbb{E}_{x \sim \mu} [F(x)]$$

for some given function  $F$  and some known distribution  $\mu$  over the set  $\mathcal{X}$ . If the expectation cannot be computed directly, we can instead approximate the value of  $f$  by the *sample mean*,

$$f \approx \frac{1}{N} \sum_{n=1}^N F(x_n),$$

where the samples  $x_1, \dots, x_N$  are distributed according to  $\mu$ . However, in many practical situations, the sample set  $S_N = \{x_1, \dots, x_N\}$  cannot easily be obtained from  $\mu$ .

MCMC methods are used to obtain samples from distributions that are hard to sample directly, and is used abundantly in statistics, optimization and machine learning for integration. The key idea behind MCMC is to build an ergodic Markov chain having  $\mu$  as the stationary distribution. The chain will eventually converge to  $\mu$ , providing a natural process to obtain samples distributed according to  $\mu$ .

This section discusses the two variations of MCMC—the Metropolis-Hastings algorithm and Gibbs samplers. However, before going into these methods in detail,

we introduce a simple property used to determine whether a distribution is the stationary distribution for a given Markov chain.

### 2.4.1 Reversibility

Often, the stationary distribution for a Markov chain  $(\mathcal{X}, \mathbf{P})$  can easily be determined by using an artifact known as *reversibility*.

#### Reversible chain

An  $(\psi)$ -irreducible positive chain  $(\mathcal{X}, \mathbf{P})$  with stationary distribution  $\mu^*$  is *reversible* if, for every  $x, y \in \mathcal{X}$ ,

$$\mu^*(x)\mathbf{P}(y | x) = \mu^*(y)\mathbf{P}(x | y). \quad (2.17)$$

In a reversible Markov chain, the time index can be reversed without affecting the dynamics of the process. Equation 2.17 is known as the *detailed balance* equation, and can be used directly to determine whether a candidate distribution  $\mu$  is the stationary distribution for a given Markov chain, requiring only the latter to be  $(\psi)$ -irreducible.

**Proposition 2.8** (Reversibility condition). *Let  $\mathcal{M} = (\mathcal{X}, \mathbf{P})$  denote a  $(\psi)$ -irreducible Markov chain and  $\mu$  a probability distribution over  $\mathcal{X}$ . If*

$$\mu(x)\mathbf{P}(y | x) = \mu(y)\mathbf{P}(x | y).$$

*for all  $x, y \in \mathcal{X}$ , then  $\mathcal{M}$  is a positive recurrent reversible chain with stationary distribution  $\mu$ .*

*Proof.* The proof is left as an exercise (Exercise 2.5). □

### 2.4.2 The Metropolis-Hastings algorithm

The first MCMC algorithm that we discuss is known as the *Metropolis-Hastings algorithm*, named after its proposers, Metropolis et al. (1953) and Hastings (1970). As with all MCMC algorithms, Metropolis-Hastings constructs a Markov chain whose stationary distribution corresponds precisely to the distribution we wish to sample. The process used to construct such a chain relies on the principle of *rejection sampling*, that we discuss in the continuation.

#### Rejection sampling

Rejection sampling is a standard approach used to generate samples from a target distribution that is hard to sample directly. Recall that we wish to generate a sample set  $S_N = \{x_1, \dots, x_N\}$  distributed according to a target distribution  $\mu$  over

some set  $\mathcal{X}$ . Sampling  $\mu$  directly is difficult. We instead pick an auxiliary distribution  $\nu$  that can easily be sampled (e.g., the uniform or the Gaussian distributions). We call  $\nu$  the *proposal distribution*, and assume that  $\nu$  verifies, for every  $x \in \mathcal{X}$ ,

$$\mu(x) \leq K\nu(x), \quad (2.18)$$

for some  $K < \infty$ .

---

**Algorithm 2.1** Rejection sampling.

---

**Require:** Target distribution,  $\mu$

**Require:** Proposal distribution,  $\nu$ , verifying (2.18)

1: Initialize  $S_N = \emptyset$

2: Initialize  $n \leftarrow 0$

3: **while**  $n < N$  **do**

4:     Sample  $x \in \mathcal{X}$  according to  $\nu$

5:     Sample  $u \in [0, 1]$  according to  $\text{Uniform}([0, 1])$

6:     Let

$$\gamma(x) = \frac{\mu(x)}{K\nu(x)},$$

7:     **if**  $u < \gamma(x)$  **then**

8:          $S_N \leftarrow S_N \cup \{x\}$

9:          $n \leftarrow n + 1$

10:     **end if**

11: **end while**

12: **return**  $S_N$

---

Rejection sampling is summarized in Algorithm 2.1. The algorithm produces a set of samples,  $S_N$ , where each sample is distributed according to  $\mu$ . Each sample in  $S_N$  is obtained by first drawing a sample  $x$  of a r.v.  $x$  distributed according to  $\nu$ . The sampled  $x$  is then accepted with probability  $\gamma(x)$ , as seen in lines 7 through 10. We have that

$$\begin{aligned} \mathbb{P}_{x \sim \nu} [x \text{ is accepted}] &= \mathbb{P}_{x \sim \nu} [u < \gamma(x)] \\ &= \int_{\mathcal{X}} \mathbb{P} \left[ u < \frac{\mu(x)}{K\nu(x)} \right] \nu(x) dx \\ &= \int_{\mathcal{X}} \frac{\mu(x)}{K\nu(x)} \nu(x) dx = \frac{1}{K}. \end{aligned}$$

But then, letting  $y$  denote the r.v. corresponding to an accepted sample from Algorithm 2.1, for any  $U \subset \mathcal{X}$ ,

$$\begin{aligned} \mathbb{P} [y \in U] &= \mathbb{P} [x \in U \mid x \text{ is accepted}] \\ &= \frac{\mathbb{P} [x \in U, x \text{ is accepted}]}{\mathbb{P} [x \text{ is accepted}]} \\ &= K \int_U \mathbb{P} \left[ u < \frac{\mu(x)}{K\nu(x)} \right] \nu(x) dx \\ &= \int_U \mu(x) dx, \end{aligned}$$

implying that  $y$  is distributed according to  $\mu$ , as desired. Unfortunately, in many practical situations, the constant  $K$  in (2.18) may be quite large, making the acceptance probability quite small and the rejection sampling approach quite slow.

### Metropolis-Hastings

Metropolis-Hastings (MH) uses the same underlying principle of rejection sampling to construct a Markov chain in which the stationary distribution corresponds to the target distribution  $\mu$ . To describe the algorithm, we depart from a proposal conditional distribution  $\nu$ , used to generate new samples from the previous ones (hence the Markov nature of the algorithm). The new sample is accepted with a probability that depends both on  $\mu$  and on  $\nu$ .

Metropolis-Hastings is summarized in Algorithm 2.2. One of the key advantages of MH is that, unlike rejection sampling, every iteration of the algorithm generates a new sample. Therefore, MH is significantly more efficient.

---

**Algorithm 2.2** The Metropolis-Hastings algorithm.

---

**Require:** Target distribution,  $\mu$

**Require:** Proposal conditional distribution,  $\nu$

**Require:** Initial value  $x_0$

```

1: Initialize  $S_N \leftarrow \{x_0\}$ 
2: Initialize  $n \leftarrow 0$ 
3: while  $n < N$  do
4:   Sample  $x \in \mathcal{X}$  according to  $\nu(\cdot \mid x_n)$ 
5:   Sample  $u \in [0, 1]$  according to  $\text{Uniform}([0, 1])$ 
6:   Let

```

$$\gamma(x \mid x_n) = \min \left\{ 1, \frac{\mu(x)\nu(x_n \mid x)}{\mu(x_n)\nu(x \mid x_n)} \right\} \quad (2.19)$$

```

7:   if  $u < \gamma(x \mid x_n)$  then
8:      $x_{n+1} \leftarrow x$ 
9:   else
10:     $x_{n+1} \leftarrow x_n$ 
11:   end if
12:    $n \leftarrow n + 1$ 
13: end while
14: return  $S_N$ 

```

---

One key aspect of MH is that the proposal distribution,  $\nu$ , is a *conditional distribution*. At each iteration  $n$ , the sample generated from  $\nu$  depends on the previous sample,  $x_{n-1}$ . Therefore, the process used to generate the samples  $\{x_0, \dots, x_N\}$  is a Markov chain with state space  $\mathcal{X}$  and transition probabilities given by

$$\begin{aligned} \mathbb{P}[x_{n+1} \in U \mid x_n = x] \\ = \mathbb{P}[x_{n+1} \in U, \lambda_\nu(x) \mid x_n = x] + \mathbb{P}[x_{n+1} \in U, \neg \lambda_\nu(x) \mid x_n = x], \end{aligned} \quad (2.20)$$

for any  $U \subset \mathcal{X}$ , where  $\lambda_\nu(x)$  is the event that a sample generated from  $x$  according to  $\nu$  was accepted and  $\neg \lambda_\nu(x)$  is the complementary event. We can further break

down (2.20) to get

$$\begin{aligned} \mathbb{P}[x_{n+1} \in U \mid x_n = x] &= \int_U \nu(y \mid x) \gamma(y \mid x) dy + \int_{\mathcal{X}} \nu(y \mid x) (1 - \gamma(y \mid x)) \mathbb{I}[x \in U] dy = \\ &= \int_U \left[ \nu(y \mid x) \gamma(y \mid x) + \delta_x(y) \left( 1 - \int_{\mathcal{X}} \nu(x' \mid x) \gamma(x' \mid x) dx' \right) \right] dy, \end{aligned}$$

where  $\delta_x(y)$  is the Dirac delta centered in  $x$ . The transition probability kernel is, thus,

$$P(y \mid x) = \nu(y \mid x) \gamma(y \mid x) + \delta_x(y) (1 - \rho(x)),$$

where

$$\rho(x) = \int_{\mathcal{X}} \nu(x' \mid x) \gamma(x' \mid x) dx'.$$

To establish that the MH Markov chain converges to the desired distribution, we note that, if  $\gamma(y \mid x) < 1$ , then  $\gamma(x \mid y) = 1/\gamma(y \mid x) = 1$  and vice-versa. Hence, without loss of generality, let us suppose that  $\gamma(y \mid x) < 1$ . Then,

$$\mu(x) \nu(y \mid x) \gamma(y \mid x) = \mu(y) \nu(x \mid y) = \mu(y) \nu(x \mid y) \gamma(x \mid y).$$

On the other hand, it is immediate that

$$\delta_x(y) \mu(x) (1 - \rho(x)) = \delta_y(x) \mu(y) (1 - \rho(y)).$$

We just showed that the Markov chain verifies the detailed balance equation

$$\mu(x) P(y \mid x) = \mu(y) P(x \mid y),$$

which implies that, in fact,  $\mu$  is the stationary distribution for the chain (see Proposition 2.8). In fact, under mild conditions (for example, if  $\nu(y \mid x) > 0$  for all  $x, y \in \mathcal{X}$ ) it can be shown that the chain verifies all conditions of Theorem 2.7 (G. Roberts and Tweedie, 1996; Tierney, 1994), which guarantees the convergence of the samples to the desired distribution.

---

**Example 2.6** We used the Metropolis-Hastings algorithm to obtain samples from a mixture of two Gaussians, as depicted in in Fig. 2.11. In particular,

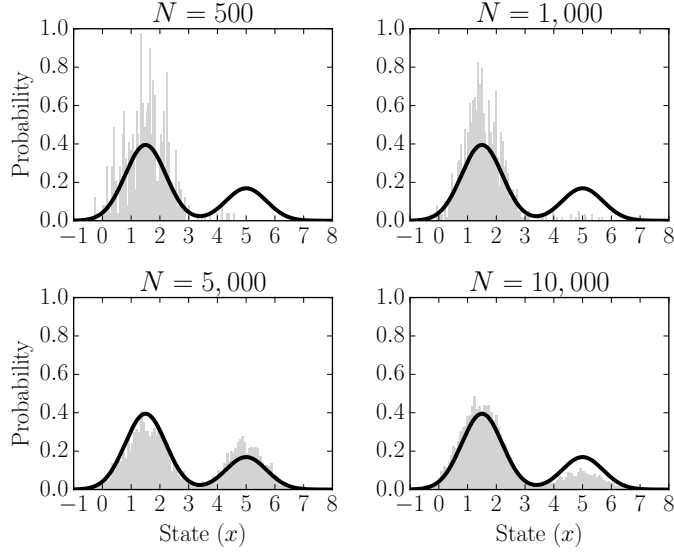
$$\mu(x) = 0.7 \mathcal{N}(x; 1.5, 1.5) + 0.3 \mathcal{N}(x; 5, 1),$$

where we write  $\text{Normal}(x; \mu, \sigma^2)$  to denote the Normal distribution with mean  $\mu$  and variance  $\sigma^2$ . We used as proposal distribution

$$\nu(y \mid x) = \mathcal{N}(y; x, 1),$$

which has the appealing property of being symmetric in the roles of  $x$  and  $y$ , which greatly facilitates the computation of the term  $\gamma(y \mid x)$  in the algorithm. The results are depicted in Fig. 2.11 for different values of  $N$ .





**Figure 2.11** Histogram of the samples obtained with Metropolis-Hastings compared with the target distribution, for  $N = 500$ ,  $N = 1,000$ ,  $N = 5,000$ , and  $N = 10,000$  samples.

### 2.4.3 Gibbs sampling

Let us now suppose that we wish to generate a sample set  $S_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  distributed according to a target distribution  $\mu$  over some set  $\mathcal{X}$ , where now  $\mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_K$  and each  $\mathcal{X}_k$  is a general set. In other words, each sample  $\mathbf{x}_n, n = 1, \dots, N$ , is a vector in which the  $k$ th component verifies  $x_{k,n} \in \mathcal{X}_k$ . As before, we are interested in the situation where directly obtaining samples from  $\mu$  is difficult. However, we now assume that it is easy to obtain samples from the conditional distributions  $\mu_k(\cdot \mid \mathbf{x}_{-k}), k = 1, \dots, K$ , where we write  $\mathbf{x}_{-k}$  to denote the vector obtained from  $\mathbf{x}$  by removing the  $k$ th component. In other words,

$$\mu_k(x_k \mid \mathbf{x}_{-k}) \stackrel{\text{def}}{=} \frac{\mu(x_1, \dots, x_k, \dots, x_K)}{\int_{\mathcal{X}_k} \mu(x_1, \dots, x'_k, \dots, x_K) dx'_k}.$$

The distributions  $\mu_k$  are known as *full conditionals*, and we can take advantage of these to obtain samples from the distribution  $\mu$  by building a Markov chain with  $\mu$  as its stationary distribution.

The *Gibbs sampler* is summarized in Algorithm 2.3. At each iteration, the algorithm randomly selects a component  $k \in \{1, \dots, K\}$  and generates a new sample by sampling  $x_k$  from the full conditional  $\mu_k$ . The resulting process is clearly a Markov chain with state space  $\mathcal{X}$  and transition probabilities given by

$$\mathbb{P}[\mathbf{x}_{n+1} \in U \mid \mathbf{x}_n = \mathbf{x}] = \sum_{k=1}^K \mathbb{P}[\mathbf{x}_{n+1} \in U \mid \mathbf{x}_n = \mathbf{x}, \lambda_k] \mathbb{P}[\lambda_k \mid \mathbf{x}_n = \mathbf{x}]$$

---

**Algorithm 2.3** The Gibbs sampler.

**Require:** Full conditional distributions,  $\mu_1, \dots, \mu_K$ 
**Require:** Initial value  $\mathbf{x}_0$ 

```

1: Initialize  $S_N \leftarrow \{\mathbf{x}_0\}$ 
2: Initialize  $n \leftarrow 0$ 
3: while  $n < N$  do
4:   Sample  $k \in \{1, \dots, K\}$  according to  $\text{Uniform}(\{1, \dots, K\})$ 
5:   Sample  $\mathbf{x} \in \mathcal{X}$  according to  $\mu_k(\cdot \mid \mathbf{x}_{-k,n})$ 
6:    $\mathbf{x}_{n+1} \leftarrow \mathbf{x}$ 
7:    $n \leftarrow n + 1$ 
8: end while
9: return  $S_N$ 

```

---

for any  $A \subset \mathcal{X}$ , where  $\lambda_k$  is the event that the component  $k$  was selected in line 4 of the algorithm. Expanding the probabilities on the righthand side, we get

$$\begin{aligned} \mathbb{P}[\mathbf{x}_{n+1} \in U \mid \mathbf{x}_n = \mathbf{x}] &= \frac{1}{K} \sum_{k=1}^K \mathbb{P}[\mathbf{x}_{n+1} \in U \mid \mathbf{x}_n = \mathbf{x}, \lambda_k] \\ &= \frac{1}{K} \int_U \sum_{k=1}^K \mu_k(y_k \mid \mathbf{x}_{-k}) \delta_{\mathbf{x}_{-k}}(\mathbf{y}_{-k}) d\mathbf{y} \end{aligned}$$

which finally yields the kernel

$$\mathbf{P}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{K} \sum_{k=1}^K \mu_k(y_k \mid \mathbf{x}_{-k}) \delta_{\mathbf{x}_{-k}}(\mathbf{y}_{-k}).$$

We can, once again, resort to the detailed balance equation to show that the Markov chain has  $\mu$  as the stationary distribution. For any  $k = 1, \dots, K$ , we have that

$$\mu(\mathbf{x}) = \mu_k(x_k \mid \mathbf{x}_{-k}) \int_{\mathcal{X}_k} \mu(z_k, \mathbf{x}_{-k}) dz_k.$$

But then,

$$\begin{aligned} \mu(\mathbf{x}) \mathbf{P}(\mathbf{y} \mid \mathbf{x}) &= \frac{1}{K} \sum_{k=1}^K \mu_k(x_k \mid \mathbf{x}_{-k}) \int_{\mathcal{X}_k} \mu(z_k, \mathbf{x}_{-k}) \mu_k(y_k \mid \mathbf{x}_{-k}) \delta_{\mathbf{x}_{-k}}(\mathbf{y}_{-k}) dz_k \\ &= \frac{1}{K} \sum_{k=1}^K \mu_k(x_k \mid \mathbf{y}_{-k}) \int_{\mathcal{X}_k} \mu(z_k, \mathbf{y}_{-k}) \mu_k(y_k \mid \mathbf{y}_{-k}) \delta_{\mathbf{y}_{-k}}(\mathbf{x}_{-k}) dz_k \\ &= \mu(\mathbf{y}) \mathbf{P}(\mathbf{x} \mid \mathbf{y}), \end{aligned}$$

where the second equality follows from the properties of the Dirac delta.

## 2.5 Bibliographical notes

The fundamental results on stability presented herein were established in the works of Kendall (1959), Vere-Jones (1962), and Popov (1977), for countable state space

chains and then extended to general state space chains by Nummelin and Tweedie (1978), among others.

Our presentation of Markov chains essentially follows the book of Meyn and Tweedie (2009). The book is a fundamental reference on the general theory of Markov chains, providing a rather broad historical perspective on how the theory was established, a plethora of methods to establish stability of Markov chains, and numerous examples and extensive discussion. A significant part of the book is devoted to the concept of stability in Markov chains, culminating in powerful criteria for the uniform ergodicity of Markov chains in general state spaces. Another good reference is the monograph by Nummelin (1984).

Section 2.4 follows Robert and Casella (1999). Markov chain Monte Carlo algorithms are extremely popular in optimization, statistics and machine learning, and date back to the 1950s and the works of Metropolis et al. (1953) and Hastings (1970). The Gibbs sampler in Section 2.4.3 is more accurately named *random sweep Gibbs sampler*, since the algorithm randomly cycles between the different full conditionals. It was originally proposed by J. Liu, Wong, and Kong (1995). More general versions exist of the Gibbs sampler exist, but establishing the properties of those versions requires a significantly more demanding analysis Robert and Casella, 1999. The original Gibbs sampler was proposed by S. Geman and D. Geman (1984). Other good references on MCMC include the articles of Andrieu et al. (2003) and G. Roberts and Rosenthal (2004), and the monograph of Häggström (2002).

## 2.6 Proofs

This section collects the proofs of the results used throughout the text.

### Proof of Lemma 2.2

As seen in Section 2.2.1, if  $(\mathcal{X}, \mathbf{P})$  is an irreducible aperiodic chain, then for any  $x, y \in \mathcal{X}$  there is  $T > 0$  such that  $\mathbf{P}^t(y | x) > 0$  for all  $t > T$ . For one such  $T$ , let  $p = \min \{ \mathbf{P}^T(y | x), x, y \in \mathcal{X} \}$ . Then,

$$\mathbb{P} [T_y > T \mid x_0 = x] \leq \mathbb{P} [x_T \neq y \mid x_0 = x] \leq 1 - p.$$

Similarly, have

$$\mathbb{P} [T_y > 2T \mid x_0 = x] = \mathbb{P} [T_y > 2T \mid T_y > T, x_0 = x] \mathbb{P} [T_y > T \mid x_0 = x] \leq (1 - p)^2$$

or, more generally,

$$\mathbb{P} [T_y > kT \mid x_0 = x] \leq (1 - p)^k.$$

Taking the limit as  $k \rightarrow \infty$ , it follows that  $\mathbb{P} [T_y = \infty \mid x_0 = x] = 0$ .

As for the second statement, we have that

$$\begin{aligned}
 \mathbb{E} [T_y \mid x_0 = x] &= \sum_{t=0}^{\infty} \mathbb{P} [T_y > t \mid x_0 = x] = \sum_{k=0}^{\infty} \sum_{t=kT}^{(k+1)T} \mathbb{P} [T_y > t \mid x_0 = x] \\
 &\leq \sum_{k=0}^{\infty} \sum_{t=kT}^{(k+1)T} \mathbb{P} [T_y > kT \mid x_0 = x] \leq T \sum_{k=0}^{\infty} \mathbb{P} [T_y > kT \mid x_0 = x] \\
 &\leq T \sum_{k=0}^{\infty} (1-p)^k = \frac{T}{p} < \infty.
 \end{aligned}$$

### Proof of Lemma 2.4

As in the proof of Lemma 2.2, since  $\mathcal{M}$  is irreducible and aperiodic, let  $T$  be such that  $\mathbf{P}^t(y \mid x) > 0$  for all  $t > T$ , and let  $p = \min \{ \mathbf{P}^T(y \mid x), x, y \in \mathcal{X} \}$ . Then,

$$\mathbb{P} [T_M \leq T] \geq \mathbb{P} [x_T = y_T] \geq \mathbb{P} [x_T = x^*, y_T = x^*],$$

for some  $x^* \in \mathcal{X}$ . In virtue of the independence of  $\mathcal{M}$  and  $\mathcal{M}'$ ,

$$\begin{aligned}
 \mathbb{P} [x_T = x^*, y_T = x^*] &= \mathbb{P} [x_T = x^*] \mathbb{P} [y_T = x^*] \\
 &= \sum_{x, y \in \mathcal{X}} \mathbb{P} [x_T = x^* \mid x_0 = x] \mathbb{P} [x_0 = x] \mathbb{P} [y_T = x^* \mid y_0 = y] \mathbb{P} [y_0 = y] \geq p^2,
 \end{aligned}$$

and  $\mathbb{P} [T_M > T] < 1 - p^2$ . Similarly, we get that  $\mathbb{P} [T_M > 2T] < (1 - p^2)^2$  or, more generally,

$$\mathbb{P} [T_M > kT] < (1 - p^2)^k.$$

Taking the limit as  $k \rightarrow \infty$ , the conclusion follows.

## 2.7 Exercises

### Exercise 2.1.

Given a Markov chain  $(\mathcal{X}, \mathbf{P})$ , show that *communication* is an equivalence relation, i.e., given any  $x, y, z \in \mathcal{X}$ ,

- It is *reflexive*, i.e.,  $x \leftrightarrow x$ ;
- It is *symmetric*, i.e., if  $x \leftrightarrow y$  then  $y \leftrightarrow x$ ;
- It is *transitive*, i.e., if  $x \leftrightarrow y$  and  $y \leftrightarrow z$  then  $x \leftrightarrow z$ .

**Exercise 2.2.**

Let  $(\mathcal{X}, \mathbf{P})$  denote an aperiodic Markov chain. Show that there is  $T < \infty$  such that

$$\mathbf{P}^t(x \mid x) > 0$$

for all  $t > T$  and all  $x \in \mathcal{X}$ .

**Suggestion:** Use the following result from number theory: if  $\mathcal{M}$  is a non-empty set of positive integers such that  $\gcd \mathcal{M} = 1$  and, given any  $i, j \in \mathcal{M}$ ,  $i + j \in \mathcal{M}$ , there is an integer  $N < \infty$  such that  $n \in \mathcal{M}$ , for all  $n > N$ .

**Exercise 2.3.**

Given a Markov chain  $(\mathcal{X}, \mathbf{P})$ , show that if  $x \leftrightarrow y$ , then  $d_x = d_y$ , where  $d_x$  denotes the period of state  $x$ .

**Exercise 2.4.**

Let  $(\mathcal{X}, \mathbf{P})$  denote an irreducible aperiodic Markov chain. Show that the corresponding stationary distribution is unique.

**Suggestion:** Use a contradiction argument. Assume that there are two distinct stationary distributions and show that, by Theorem 2.3, the two must be the same.

**Exercise 2.5.**

Prove Proposition 2.8.