Lecture 3: Discrete-Time Markov Chain Models

1 One-Step Transition Probabilities

Let us consider a system that can be in any one of a finite or countably infinite number of states, and let Ψ denote this set of states, where we assume that $\Psi \in \mathbb{Z}$ (or, that Ψ is a subset of the integers). The set Ψ is called the **state space** of the system. Let the system be observed at discrete time points $n = 0, 1, 2, \cdots$, and let X_n denote the state of the system at time n. We can also think of X_n as random variables defined on a common probability space. Then, $\{X_n,\ n = 0, 1, 2, \cdots\}$ is a discrete stochastic process that takes on a countable number of possible values. When

$$X_n = i \,,$$

then the process is said to be in state i at time n.

Suppose that whenever the process in state i, it will be next in state j with a fixed probability P_{ij}. That is,

$$\begin{aligned} P\{X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \cdots, X_1 = i_1, X_0 = i_0\} &= P\{X_{n+1} = j | X_n = i\} \\ &= P_{ij} \,, \end{aligned} \tag{1}$$

for all states $i_0, i_1, \cdots, i_{n-1}, i, j \geq 0$ and all set of times $n+1 > n > \cdots \geq 0$.

Such a stochastic process is known as a **Markov chain** and equation (1) is called the **Markov property**.

Equation (1) states that, for a Markov chain, given the present state X_n, the conditional distribution of any future state X_{n+1} is independent of the past states $X_{n-1}, X_{n-2}, \cdots$ and depends only on the present state X_n.

The Markov property is sometimes referred to as the 'memoryless' property.

The conditional probabilities $P\{X_{n+1} = j | X_n = i\}$ are called the **transition probabilities** of the chain. The value P_{ij} represents the probability that when in state i, the process will next make a transition into state j, and it satisfies the conditions:

- Probabilities are nonnegative,

$$P_{ij} \geq 0\,, \qquad \text{for } i, j = 0, 1, 2, \cdots$$

- Probabilities sum to one,

$$\sum_{j=0}^{\infty} P_{ij} = 1\,, \qquad \text{for } i = 0, 1, 2, \cdots$$

The probability distribution of state transitions is typically represented as the **Markov chain's transition probability matrix** whose entries in each row must add up to exactly one. The matrix of one-step transition probabilities P_{ij} is given by,

$$\mathbf{P} = \begin{bmatrix} P_{00} & P_{01} & P_{02} & \cdots \\ P_{10} & P_{11} & P_{12} & \cdots \\ \vdots & \vdots & \vdots & \\ P_{i0} & P_{i1} & P_{i2} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{2}$$

Example 3.1: Two-State Markov Chain

A simple molecular switch can be considered an example of a Markov chain having two states. An example of the molecular switch are ligand-gated ionic channels, also called ionotropic receptors, which are transmembrane ion-channel proteins which open and close to allows ions such as Na^+, K^+, Ca^{2+}, and/or Cl^- to pass through the cell membrane in response to the binding of a cell to a ligand [5]. Here we model proteins that are switching between an "open" state and a "closed" state, and nothing more at this point. Suppose also that if the channel is now open, then it will next be open with probability α; and if it is now closed, then it will next be open with probability β.

If we say that the process is in state,

0 when it open,

1 when it closed,

then it is a two-state Markov chain, where the elements of the transition probabilities matrix based on the above description are,

if the channel is now open, it will next be open with probability α: $\rightarrow P_{00} = \alpha$

if the channel is now closed, it will next be open with probability β: $\rightarrow P_{10} = \beta$

and it follows immediately that,

if the channel is now open, it will next be closed with probability $1-\alpha$: $\rightarrow P_{01} = 1-\alpha$

if the channel is now closed, it will next be closed with probability $1-\beta$: $\rightarrow P_{11} = 1-\beta$

Alternatively, we can arrange the transition probabilities in a table,

		Next State	
		Open "0"	Closed "1"
Current State	Open "0"	α	$1-\alpha$
	Closed "1"	β	$1-\beta$

A transition diagram for this example is shown in Fig. 1.

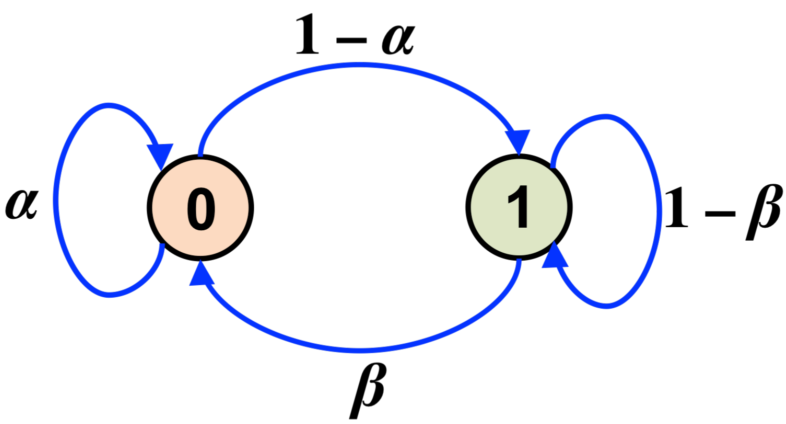

Figure 1: A transition diagram for the two-state Markov chain of the simple molecular switch example.

Hence the transition probability matrix of the two-state Markov chain is,

$$\mathbf{P} = \begin{bmatrix} P_{00} & P_{01} \\ P_{10} & P_{11} \end{bmatrix} = \begin{bmatrix} \alpha & 1-\alpha \\ \beta & 1-\beta \end{bmatrix}$$

Notice that the sum of the first row of the transition probability matrix is $\alpha + (1-\alpha)$ or equal to 1. Similarly for the second row.

Example 3.2: Four-State Markov Chain

This example is taken from **Example 4.4 in** [4]**:**
(Transforming a Process into a Markov Chain) Suppose that whether or not it rains today

depends on previous weather conditions through the last two days. Specifically, suppose that if it has rained for the past two days, then it will rain tomorrow with probability 0.7; if it rained today but not yesterday, then it will rain tomorrow with probability 0.5; if it rained yesterday but not today, then it will rain tomorrow with probability 0.4; if it has not rained in the past two days, then it will rain tomorrow with probability 0.2.

The state of this model at any time is determined by the weather conditions during both that day and the previous day. In other words, we can say that the process is in,

- state 0 (S_0): if it rained both today and yesterday,
- state 1 (S_1): if it rained today but not yesterday,
- state 2 (S_2): if it rained yesterday but not today,
- state 3 (S_3): if it did not rain either yesterday or today.

and the states for tomorrow's weather conditions,

- state 00 (S_{00}): tomorrow will rain if it rained today and yesterday $\rightarrow P_{00} = 0.7$,
- state 10 (S_{10}): tomorrow will rain if it rained today but not yesterday $\rightarrow P_{10} = 0.5$,
- state 21 (S_{21}): tomorrow will rain if it rained yesterday but not today $\rightarrow P_{21} = 0.4$,
- state 31 (S_{31}): tomorrow will rain if it did not rain yesterday or today $\rightarrow P_{31} = 0.2$.

It follows immediately that,

- state 02 (S_{02}): tomorrow won't rain if it rained today and yesterday $\rightarrow P_{02} = 1-0.7 = 0.3$,
- state 12 (S_{12}): tomorrow won't rain if it rained today but not yesterday $\rightarrow P_{12} = 1-0.5 = 0.5$,
- state 23 (S_{23}): tomorrow won't rain if it rained yesterday but not today $\rightarrow P_{23} = 1-0.4 = 0.6$,
- state 33 (S_{33}): tomorrow won't rain if it did not rain either yesterday or today $\rightarrow P_{33} = 1-0.2 = 0.8$.

These state transitions may be better explained in a tree diagram, as shown in Fig. 2.

Or, its transition diagram can be seen in Fig. 3.

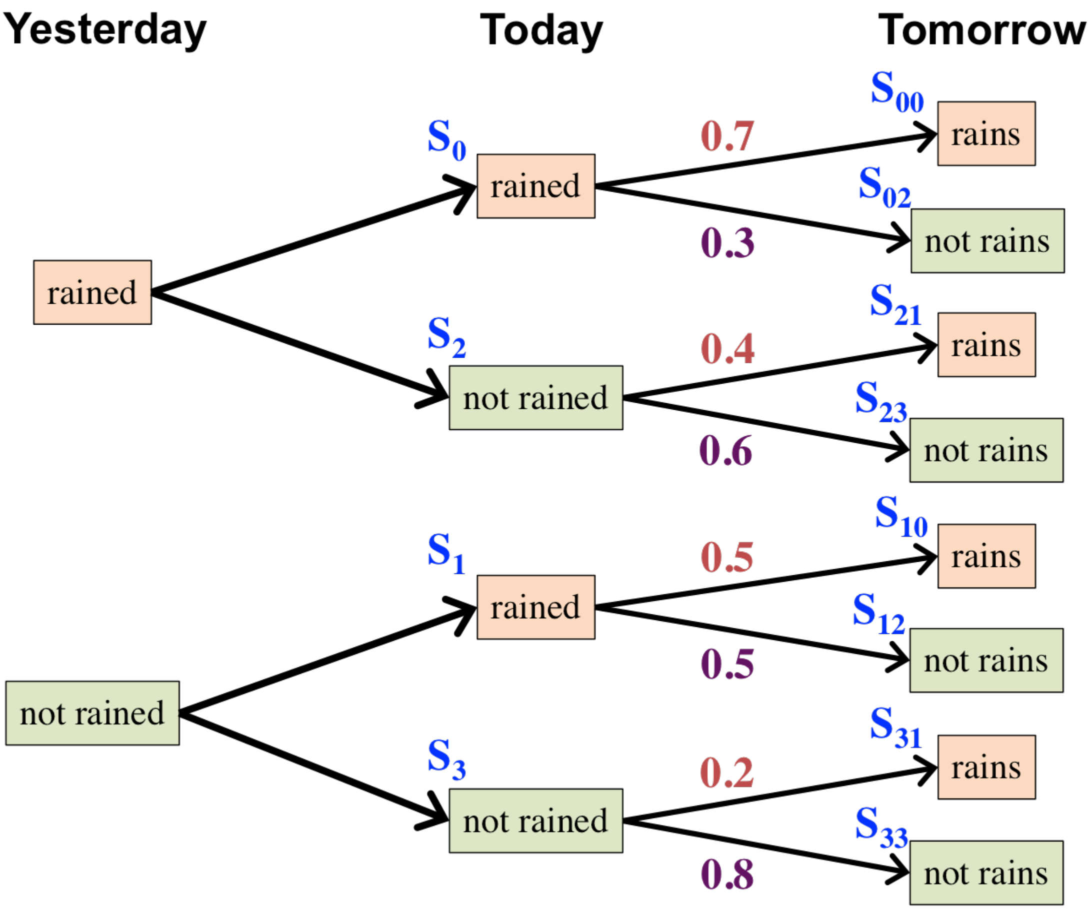

Figure 2: A tree diagram for the four-state Markov chain example.

The transition probability matrix of the four-state Markov chain is,

$$\mathbf{P} = \begin{bmatrix} P_{00} & P_{01} & P_{02} & P_{03} \\ P_{10} & P_{11} & P_{12} & P_{13} \\ P_{20} & P_{21} & P_{22} & P_{23} \\ P_{30} & P_{31} & P_{32} & P_{33} \end{bmatrix} = \begin{bmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{bmatrix}$$

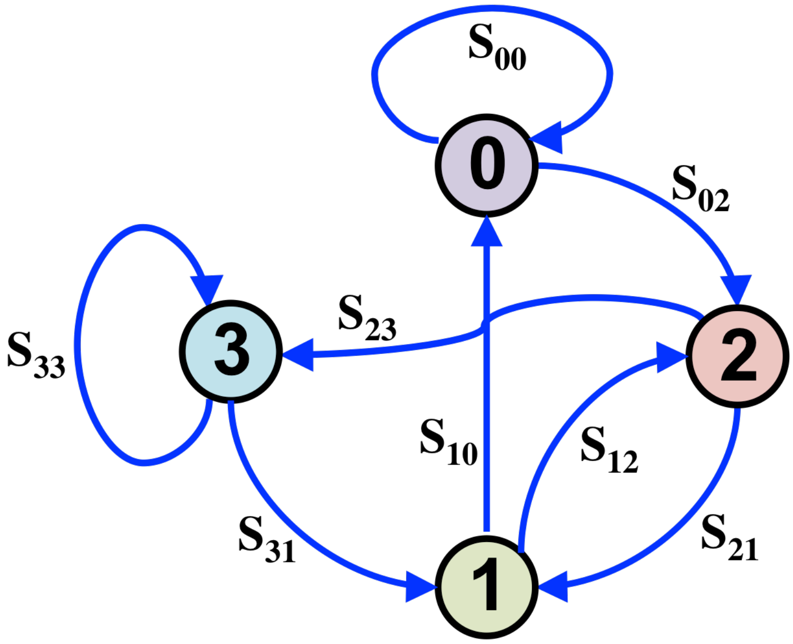

Figure 3: A transition diagram for the four-state Markov chain of the weather forecast example.

2 n-Step Transition Probabilities

A Markov chain is completely defined by its one-step transition probability matrix and the specification of a probability distribution on the state of the process at time 0 (which, we can also think of it as initial conditions). The analysis of a Markov chain is mainly about the calculation of the probabilities of the possible $\{X_n\}$ of the process. Central in these calculations are the n-step transition probabilities [3].

The n-step transition probabilities P_{ij}^n of a Markov chain is the probability that a process in state i will be in state j after n additional transitions. These probabilities satisfy,

$$P_{ij}^n = P\{X_{n+k} = j \,|\, X_k = i\}\,, \qquad n \geq 0\,, \quad i, j \geq 0 \tag{3}$$

with several cases:

- $n = 0$
  Following conditional probabilities,

$$P_{ij}^0 = \delta_{ij} = \begin{cases} 1 & \text{if } \; i = j\,, \\ 0 & \text{if } \; i \neq j\,. \end{cases}$$

- $n = 1$
  It is the case of one-step transition probabilities that we have discussed in the previous section, where $P_{ij}^1 = P_{ij}$.

- $n > 1$
  It is the case of n-step transition probabilities. To compute these probabilities, the **Chapman-Kolmogorov equations** are used. These equations are formulated,

$$P_{ij}^{n+m} = \sum_{k=0}^{\infty} P_{ik}^{n} P_{kj}^{m}\,, \qquad \text{for } n, m \geq 0, \text{ all } i, j \tag{4}$$

Verification of the Chapman-Kolmogorov equations can be shown as follows,

$$\begin{aligned} P_{ij}^{n+m} &= P\{X_{n+m} = j \,|\, X_0 = i\} \\ &= \sum_{k=0}^{\infty} P\{X_{n+m} = j, X_n = k \,|\, X_0 = i\}\,. \end{aligned} \tag{5}$$

Following conditional probabilities, equation (5) becomes

$$P_{ij}^{n+m} = \sum_{k=0}^{\infty} P\{X_{n+m} = j \,|\, X_n = k, X_0 = i\}\, P\{X_n = k \,|\, X_0 = i\}\,. \tag{6}$$

Following the Markov property, equation (6) now

$$\begin{aligned} P_{ij}^{n+m} &= \sum_{k=0}^{\infty} P\{X_{n+m} = j \,|\, X_n = k\}\, P\{X_n = k \,|\, X_0 = i\} \\ &= \sum_{k=0}^{\infty} P_{kj}^{n+m-n}\, P_{ik}^{n-0} \\ &= \sum_{k=0}^{\infty} P_{kj}^{m}\, P_{ik}^{n}\,. \end{aligned} \tag{7}$$

The term $P_{ik}^{n} P_{kj}^{m}$ represents the probability that starting in i the process will go to state j in $n + m$ transitions through a path which takes it into state k at the nth transition. Summing over all intermediate states k yields the probability that the process will be in state j after $n + m$ transitions.

The preceding identity (7) written in terms of matrix notation yields matrix multiplication

$$\mathbf{P}^{(n+m)} = \mathbf{P}^{(n)} \cdot \mathbf{P}^{(m)} \tag{8}$$

where $\mathbf{P}^{(n)}$ denotes the matrix of n-step transition probabilities P_{ij}^{n}.

The transition probability matrix is given by,

- for $n = 0$:
$$\mathbf{P}^{(0)} = \mathbf{I}\,,$$
where $\mathbf{I}$ is the identity matrix.
- for $n = 1$:
$$\mathbf{P}^{(1)} = \mathbf{P}\,.$$
- for $n > 1$, it follows from the Chapman-Kolmogorov equations (8) that:
$$\mathbf{P}^{(2)} = \mathbf{P}^{(1+1)} = \mathbf{P}^{(1)} \cdot \mathbf{P}^{(1)} = \mathbf{P} \cdot \mathbf{P} = \mathbf{P}^2\,,$$
and in general,
$$\mathbf{P}^{(n)} = \mathbf{P}^{(n-1+1)} = \mathbf{P}^{n-1} \cdot \mathbf{P} = \mathbf{P}^n\,.$$
It states that the n-step transition matrix $\mathbf{P}^{(n)}$ is just the nth power of $\mathbf{P}$.

Example 3.3

Consider Example 3.1 in the previous section, in which a simple molecular switch is considered as a two-state Markov chain.

Now, we include initial distributions of the two-state Markov chain and calculate the probabilities after n steps.

Let $\pi_0(0)$ denote the probability that the channel is initially open (in state 0). That is,

$$P\{X_0 = 0\} = \pi_0(0)\,. \tag{9}$$

It follows that the probability $\pi_0(1)$ of being initially closed (in state 1) is given by,

$$\pi_0(1) = P\{X_0 = 1\} = 1 - \pi_0(0)\,.$$

From this information we can easily compute $P\{X_n = 0\}$ and $P\{X_n = 1\}$. We rewrite the transition probabilities,

$$\begin{aligned} P\{X_{n+1} = 0 \,|\, X_n = 0\} &= \alpha \\ P\{X_{n+1} = 0 \,|\, X_n = 1\} &= \beta \end{aligned} \tag{10}$$

and it follows that,

$$\begin{aligned} P\{X_{n+1} = 1 \,|\, X_n = 0\} &= 1 - \alpha\,, \\ P\{X_{n+1} = 1 \,|\, X_n = 1\} &= 1 - \beta\,. \end{aligned}$$

Using (10) and following conditional probabilities, we observe that

$$\begin{aligned} P\{X_{n+1}=0\} &= P\{X_n=0 \;\cap\; X_{n+1}=0\} + P\{X_n=1 \;\cap\; X_{n+1}=0\} \\ &= P\{X_n=0\}\, P\{X_{n+1}=0 \,|\, X_n=0\} + P\{X_n=1\}\, P\{X_{n+1}=0 \,|\, X_n=1\} \\ &= \alpha\, P\{X_n=0\} + \beta\, P\{X_n=1\} \\ &= \alpha\, P\{X_n=0\} + \beta\,(1-P\{X_n=0\}) \\ &= (\alpha-\beta)\, P\{X_n=0\} + \beta \end{aligned} \tag{11}$$

Now, using (11) and due to (9), so for $n=0$,

$$\begin{aligned} P\{X_1=0\} &= (\alpha-\beta)\, P\{X_0=0\} + \beta \\ &= (\alpha-\beta)\, \pi_0(0) + \beta\,, \end{aligned}$$

and subsequently for $n=1$,

$$\begin{aligned} P\{X_2=0\} &= (\alpha-\beta)\, P\{X_1=0\} + \beta \\ &= (\alpha-\beta)\left[(\alpha-\beta)\, \pi_0(0) + \beta\right] + \beta \\ &= (\alpha-\beta)^2\, \pi_0(0) + (\alpha-\beta)\beta + \beta\,, \end{aligned}$$

and for $n=2$,

$$\begin{aligned} P\{X_3=0\} &= (\alpha-\beta)\, P\{X_2=0\} + \beta \\ &= (\alpha-\beta)\left[(\alpha-\beta)^2\, \pi_0(0) + (\alpha-\beta)\beta + \beta\right] + \beta \\ &= (\alpha-\beta)^3\, \pi_0(0) + (\alpha-\beta)^2\beta + (\alpha-\beta)\beta + \beta\,. \end{aligned}$$

By repeating this procedure n times, we can easily obtain,

$$P\{X_n=0\} = (\alpha-\beta)^n\, \pi_0(0) + \beta \sum_{k=0}^{n-1} (\alpha-\beta)^k\,. \tag{12}$$

The same way for $P\{X_n=1\}$, we obtain,

$$P\{X_n=1\} = (\alpha-\beta)^n\, \pi_0(1) + (1-\alpha) \sum_{k=0}^{n-1} (\alpha-\beta)^k\,. \tag{13}$$

We consider the following cases to obtain the probabilities of the gate when being open and closed:

1. In the trivial case, where $\alpha = \beta = 0$, it is clear that for all n,

$$P\{X_n = 0\} = \pi_0(0)\,, \tag{14}$$

and

$$P\{X_n = 1\} = \pi_0(1)\,. \tag{15}$$

2. In the non-trivial case, where $\alpha + \beta > 0$, the expansion of the sum,

$$\sum_{k=0}^{n-1} (\alpha - \beta)^k = 1 + (\alpha - \beta) + (\alpha - \beta)^2 + (\alpha - \beta)^3 + \cdots$$

gives us a finite geometric progression, with the first term $a = 1$ and the common ratio $r = \alpha - \beta$. Thus, the sum of finite n terms, provided that $r \neq 1$, is given by,

$$S_n = \frac{a(1 - r^n)}{1 - r} = \frac{1 - (\alpha - \beta)^n}{1 - \alpha + \beta}\,.$$

Hence,

$$\begin{aligned} P\{X_n = 0\} &= (\alpha - \beta)^n \, \pi_0(0) + \beta \left(\frac{1 - (\alpha - \beta)^n}{1 - \alpha + \beta} \right) \\ &= (\alpha - \beta)^n \left(\pi_0(0) - \frac{\beta}{1 - \alpha + \beta} \right) + \frac{\beta}{1 - \alpha + \beta}\,, \end{aligned} \tag{16}$$

and consequently,

$$P\{X_n = 1\} = (\alpha - \beta)^n \left(\pi_0(1) - \frac{1 - \alpha}{1 - \alpha + \beta} \right) + \frac{1 - \alpha}{1 - \alpha + \beta}\,. \tag{17}$$

3. In another trivial case, where α and β are neither both equal to zero nor both equal to one. In this case, we can let $n \to \infty$ in (16) and (17), thus,

$$\lim_{n \to \infty} P\{X_n = 0\} = \frac{\beta}{1 - \alpha + \beta}\,, \tag{18}$$

and

$$\lim_{n \to \infty} P\{X_n = 1\} = \frac{1 - \alpha}{1 - \alpha + \beta}\,. \tag{19}$$

For a more general case of two-state Markov chain, where the transition matrix is,

		X_{n+1}	
		State 0	State 1
X_n	State 0	α	γ
	State 1	β	η

The probabilities for the next state in state 0,

$$\begin{aligned} P\{X_{n+1} = 0 \,|\, X_n = 0\} &= \alpha \\ P\{X_{n+1} = 0 \,|\, X_n = 1\} &= \beta \,, \end{aligned}$$

and the probabilities for the next state in state 1,

$$\begin{aligned} P\{X_{n+1} = 1 \,|\, X_n = 0\} &= \gamma \\ P\{X_{n+1} = 1 \,|\, X_n = 1\} &= \eta \,, \end{aligned}$$

from which, together with $P\{X_n = 0\} = \pi_0(0)$ and $P\{X_n = 1\} = \pi_0(1)$, we obtain,

$$P\{X_n = 0\} = (\alpha - \beta)^n \left(\pi_0(0) - \frac{\beta}{1 - \alpha + \beta}\right) + \frac{\beta}{1 - \alpha + \beta} \,, \tag{20}$$

and

$$P\{X_n = 1\} = (\eta - \gamma)^n \left(\pi_0(1) - \frac{\gamma}{1 - \eta + \gamma}\right) + \frac{\gamma}{1 - \eta + \gamma} \,. \tag{21}$$

Example 3.4

Consider Example 3.3 above. If $\alpha = 0.7$ and $\beta = 0.4$, calculate the probability that the channel will be open after switching 4 times given that the current state of the channel is open.

From formulations above, we know two possible ways to calculate the probability with $n = 4$:

1. By using equation (16), where $\pi_0(0) = 1$,

$$P\{X_4 = 0\} = (0.7 - 0.4)^4 \left(1 - \frac{0.4}{1 - 0.7 + 0.4}\right) + \frac{0.4}{1 - 0.7 + 0.4} = 0.5749 \,. \qquad \blacksquare$$

2. By calculating transition probability matrices.

   The one-step transition probability matrix is,

$$\mathbf{P} = \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix}$$

   Hence,

$$\mathbf{P}^{(2)} = \mathbf{P}^2 = \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix} \cdot \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{bmatrix}$$

   and for $n = 4$,

$$\mathbf{P}^{(4)} = \left(\mathbf{P}^2\right)^2 = \begin{bmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{bmatrix} \cdot \begin{bmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{bmatrix} = \begin{bmatrix} 0.5749 & 0.4251 \\ 0.5668 & 0.4332 \end{bmatrix}$$

   thus, the desired probability P_{00}^4 equals 0.5749. ■

Example 3.5

Consider Example 3.2 in the previous section. Given that it rained on Monday and Tuesday, what is the probability that it will rain on Thursday?

Given that it rained on Monday and Tuesday,

- $n = 1$ is for the probability it will rain on Wednesday,
- $n = 2$ is for the probability it will rain on Thursday,

hence $n = 2$. The two-step transition matrix is given by,

$$\begin{aligned} \mathbf{P}^{(2)} = \mathbf{P}^2 &= \begin{bmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{bmatrix} \cdot \begin{bmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{bmatrix} \\ &= \begin{bmatrix} 0.49 & 0.12 & 0.21 & 0.18 \\ 0.35 & 0.20 & 0.15 & 0.30 \\ 0.20 & 0.12 & 0.20 & 0.48 \\ 0.10 & 0.16 & 0.10 & 0.64 \end{bmatrix} \end{aligned}$$

Since rain on Thursday is equivalent to the process being in either state 0 or state 1 on Thursday, the desired probability is given by $P_{00}^2 + P_{01}^2 = 0.49 + 0.12 = 0.61$.

2.1 Unconditional Probabilities

All probabilities in previous sections are conditional probabilities, such as, P_{ij}^n is the probability that the state at time n is j given that the initial state at time 0 is i. For unconditional probabilities, the unconditional distribution of the state at time n is preferred, and it is necessary to specify the probability distribution of the initial state. Let us denote this by

$$\alpha_i \equiv P\{X_0 = i\}\,, \qquad i \geq 0 \left(\sum_{i=0}^{\infty} \alpha_i = 1 \right)$$

All unconditional probabilities may be computed by conditioning on the initial state. That is,

$$\begin{aligned} P\{X_n = j\} &= \sum_{i=0}^{\infty} P\{X_n = j \,|\, X_0 = i\}\, P\{X_0 = i\} \\ &= \sum_{i=0}^{\infty} P_{ij}^n\, \alpha_i\,. \end{aligned} \tag{22}$$

Example 3.6

For example, in the Example 3.5 above, if $\alpha_0 = 0.4$ and $\alpha_1 = 0.6$, then the unconditional probability that it will rain four days after weather records start is,

$$\begin{aligned} P\{X_4 = 0\} &= \alpha_0\, P_{00}^4 + \alpha_1\, P_{10}^4 \\ &= (0.4)(0.5749) + (0.6)(0.5668) \\ &= 0.5700 \end{aligned}$$

2.2 Classification of States

States of a Markov chain that are accessible to each other are said to communicate. Communications between the states of a Markov chain lead to a classification scheme for the states, and classification for Markov chains.

For example,

- State j is said to be accessible from state i if there is nonzero probability $P_{ij}^n > 0$ for some $n \geq 0$. This relationship is denoted as $i \to j$.
- If state i is accessible from state j, the relationship is denoted as $j \to i$, and there is $P_{ji}^{n'} > 0$ for some $n' \geq 0$.

- If states i and j are accessible to each other, $i \to j$ and $j \to i$, both states are said to communicate, or to be in the same class, denoted as $i \leftrightarrow j$.
- If two states i and j do not communicate, then either,

  $$P_{ij}^n = 0 \qquad \text{for all} \;\; n \geq 0$$

  or

  $$P_{ji}^n = 0 \qquad \text{for all} \;\; n \geq 0$$

  or both relations are true.

As in [1], the relation $i \to j$ can be represented as a directed graph, as shown in Fig. 4.

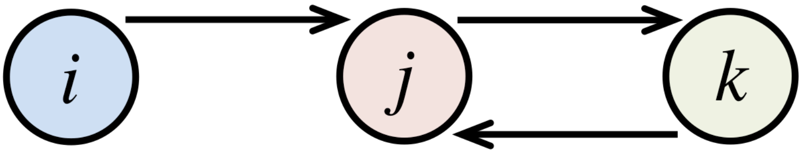

Figure 4: Directed graph where state j is accessible from state i ($i \to j$ with $P_{ij} > 0$) and state k is accessible from state i ($i \to k$ with $P_{ik}^{(2)} > 0$). On the reverse, state j is accessible from state k ($k \to j$ with $P_{kj} > 0$), but state i is not accessible from state k nor state j.

The relation of communication satisfies the following three properties:

(1) *Reflexivity*: $i \leftrightarrow i$, or state i communicates with state i. Note that for any state that communicates with itself,

$$P_{ii}^0 = P\{X_0 = i \,|\, X_0 = i\} = 1\,,$$

which is a consequence of the definition of

$$P_{ij}^0 = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Starting in state i, the system stays in state i if there is no time change. State i is also called *absorbing*.

(2) *Symmetry*: $i \leftrightarrow j$, or if state i communicates with state j, then state j communicates with state i.

(3) *Transitivity*: $i \leftrightarrow j$, $j \leftrightarrow k$ implies $i \leftrightarrow k$, or if state i communicates with state j, and state j communicates with state k, then state i communicates with state k.

Properties (1) and (2) follow from the definition of communication. To verify property (3), suppose that i communicates with j, and j communicates with k. Thus, there exist nonnegative integers n and m such that $P_{ij}^n > 0$ and $P_{jk}^m > 0$. By the Chapman-Kolmogorov equations,

$$\begin{aligned} P_{ik}^{n+m} &= P\{X_{n+m} = k \,|\, X_0 = i\} \\ &= P\{X_{n+m} = k, X_n = j \,|\, X_0 = i\} \\ &= P\{X_{n+m} = k \,|\, X_n = j\}\, P\{X_n = j \,|\, X_0 = i\} \\ &= P_{jk}^m\, P_{ij}^n > 0\,. \end{aligned} \tag{23}$$

Thus, $P_{ik}^{n+m} > 0$ and $i \to k$. Similarly, we can show that state i is accessible from state k. Hence, states i and k communicate.

Two states that communicate are said to be in the same class. The Markov chain is said to be *irreducible* if there is only one class, that is, if all states communicate with each other. But if there is more than one class, the Markov chain is said to be *reducible*. The set of equivalence classes in a discrete-time Markov chain are called the *communication classes*, or the *classes of the Markov chain* [4, 1].

Another property of a communication class is that it is *closed*. A set of states $\mathcal{C}$ is said to be closed if it is impossible to reach any state outside of $\mathcal{C}$ from any state in $\mathcal{C}$ by one-step transitions, such that,

$$P_{ij} = 0 \quad \text{if} \;\; i \in \mathcal{C} \;\; \text{and} \;\; j \notin \mathcal{C} \tag{24}$$

If in the set of states $\mathcal{C} = \{0, 1, 2, \cdots, N\}$ where probabilities of states 0 and N are $P_{00} = 1$ and $P_{NN} = 1$, respectively, these states are called *absorbing states* or *absorbing boundaries*.

2.3 Periodicity

The period of state i, denoted as $d(i)$, is defined as the greatest common advisor of all integers $n \geq 1$ for which $P_{ii}^n > 0$. Here $d(i)$ is a nonnegative integer.

- If a state i has period $d(i) > 1$, it is said to be *periodic* of period $d(i)$.
- If the period of state equals one, it is said to be *aperiodic*.
- If $P_{ii}^n = 0$ for all $n \geq 1$, then $d(i) = 0$.

In a single state i, with $P_{ii} > 0$, the state has period one.

In a finite Markov chain of n states with transition matrix

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & \ddots & & \vdots \\ 0 & 0 & & & & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix},$$

each state has period n.

Periodicity is a class property. There are three basic properties of the period of a state:

- If $i \leftrightarrow j$ then $d(i) = d(j)$. All states in one class have the same period.
- If state i has period $d(i)$ then there exists an integer N, depending on i such that for all integers $n \geq N$,
$$P_{ii}^{n\,d(i)} > 0\,.$$
This asserts that a return to state i can occur at all sufficiently large multiples of the period $d(i)$.
- If $P_{ji}^{m} > 0$, then $P_{ji}^{m+n\,d(i)} > 0$ for all n sufficiently large.

In Fig. 5, the absorbing boundaries, classes $\{0\}$ and $\{N\}$, are aperiodic. The transient class $\{1, 2, \cdots, N-1\}$ has period 2. In unrestricted random walk models, as shown in Figures. 9 and 10, the entire chain is periodic of period 2, with notation $d = 2$.

2.4 Recurrence

Consider an arbitrary but fixed, state i. We define for each integer $n \geq 1$,

$$f_{ii}^{(n)} = P\{X_n = i, X_m \neq i, m = 1, 2, \cdots, n-1 \,|\, X_0 = i\}\,, \tag{25}$$

where $f_{ii}^{(n)}$ denotes the probability that, starting from state i, the first return of a Markov chain to state i occurs at the nth transition. The probabilities $f_{ii}^{(n)}$ are also known as *first return probabilities*.

Note that,

* $f_{ii}^{(0)} = 0$ for all i,
* $f_{ii}^{(1)} = P_{ii}$,

* However, in general, $f_{ii}^{(n)} \neq P_{ii}^{(n)}$. The first return probabilities $f_{ii}^{(n)}$ may be calculated recursively according to,

$$P_{ii}^{n} = \sum_{k=0}^{n} f_{ii}^{k} \, P_{ii}^{n-k} \,, \qquad n \geq 1 \,. \tag{26}$$

To verify equation (26), consider all the possible realizations $\{X_n\}$ of the process for which $X_0 = i$, $X_n = i$ and the first return to state i occurs at the kth transition. Suppose we call this event E_k. By definition, the probability of the event that the first return is at the kth transition is f_{ii}^{k}. In the remaining $n-k$ transitions, we are dealing only with those realizations for which $X_n = i$. Using the Markov property,

$$\begin{aligned} P\{E_k\} &= P\{\text{first return is at } k\text{th transition} \,|\, X_0 = i\} \, P\{X_n = i \,|\, X_k = i\} \\ &= f_{ii}^{k} \, P_{ii}^{(n-k)} \quad \text{for } 1 \leq k \leq n \,, \end{aligned}$$

since $P_{ii}^{0} = 1$. Then,

$$P\{X_n = i \,|\, X_0 = i\} = \sum_{k=1}^{n} P\{E_k\}$$

which is equal to

$$P_{ii}^{n} = \sum_{k=1}^{n} f_{ii}^{k} \, P_{ii}^{n-k} = \sum_{k=0}^{n} f_{ii}^{k} \, P_{ii}^{n-k} \qquad \blacksquare$$

since by definition $f_{ii}^{0} = 0$.

The first return probabilities represent the *first time* the Markov chain returns to state i, thus,

$$0 \leq \sum_{n=1}^{\infty} f_{ii}^{(n)} \leq 1 \,.$$

A transient state is defined in terms of these first return probabilities:

✓ State i is said to be *recurrent* if,

$$\sum_{n=1}^{\infty} f_{ii}^{(n)} = 1 \,.$$

✓ A nonrecurrent state i is said to be *transient* if,

$$\sum_{n=1}^{\infty} f_{ii}^{(n)} < 1 \,.$$

Let T_{ii} be a random variable that defines the first return time to state i, or, we may think of T_{ii} as the time of the first visit to state i. Let

$$T_{ii} = \begin{cases} 1 & \text{if } X_n = i \\ \\ 0 & \text{if } X_n \neq i \end{cases} \tag{27}$$

If the first visit never occurs, then $T_{ii} = \infty$.

This says that,

★ Suppose that a process starts in state i and i is recurrent, then the set $\{f_{ii}^{(n)}\}_{n=0}^{\infty}$ defines a probability distribution for T_{ii}. With probability 1, $\left(\text{from } \sum_{n=1}^{\infty} f_{ii}^{(n)} = 1\right)$ the process will eventually return to state i infinitely often. An absorbing state is necessarily recurrent.

★ On the other hand, if state i is a transient state, then no matter where the Markov chain starts, it makes only a finite number of visits to state i and the expected number of visits to state i is finite. In other words, for a transient state i, if we let

$$f_{ii} = \sum_{n=0}^{\infty} f_{ii}^{(n)} < 1,$$

the Markov chain has positive probability $1 - f_{ii}$ of never returning to state i. Therefore, starting in state i, the probability that the process will be in state i for exactly n time periods is $f_{ii}^{(n-1)}\,(1 - f_{ii})\,,\ n \geq 1$.

The random variable T_{ii} may be thought of as a "waiting time" until the chain returns to state i.

The mean recurrence time to state i, denoted $\mu_{ii} = E(T_{ii})$ is defined as

$$\mu_{ii} = E(T_{ii}\,|\,X_0 = i) = \begin{cases} \sum_{n=1}^{\infty} n\, f_{ii}^{(n)} & \text{if } i \text{ is recurrent} \\ \\ \infty & \text{if } i \text{ is transient} \end{cases} \tag{28}$$

The mean recurrence time μ_{ii} for a transient state is always infinite, whereas μ_{ii} for a recurrent state can be finite or infinite [1].

For a recurrent state i,

$$i \text{ is called} = \begin{cases} \textbf{null} & \text{if } \mu_{ii} = \infty \\ \\ \textbf{non-null} \ (\text{or } \textbf{positive}) & \text{if } \mu_{ii} < \infty \end{cases}$$

An absorbing state is a simple example of a positive recurrent state with mean recurrence time $\mu_{ii} = 1$. This is a consequence of the fact that if i is an absorbing state, then $P_{ii} = 1$ implies $f_{ii}^{(1)} = 1$ and $f_{ii}^{(n)} = 0$ for $n \neq 1$.

Also, the mean recurrence time,

$$\begin{aligned}
\mu_{ii} &= E\left(\sum_{n=0}^{\infty} T_{ii} \,|\, X_0 = i\right) = \sum_{n=0}^{\infty} E\left(T_{ii} \,|\, X_0 = i\right) \\
&= \sum_{n=0}^{\infty} P\{X_n = i \,|\, X_0 = i\} \\
&= \sum_{n=0}^{\infty} P_{ii}^n
\end{aligned}$$

from which, the following has been proven:

- State i is recurrent if,
$$\sum_{n=1}^{\infty} P_{ii}^n = \infty$$
- State i is transient if,
$$\sum_{n=1}^{\infty} P_{ii}^n < \infty$$

A recurrent state i is null if and only if $P_{ii}^n \to 0$ as $n \to \infty$.

Recurrence is a class property, that is, all states in an equivalence class are either recurrent or nonrecurrent (transient).

A Markov chain is called a transient chain if all of its states are transient and a recurrent chain if all of its states are recurrent. A Markov chain having a finite state space must have at least one recurrent state and hence cannot possibly be a transient chain.

Let us now look at the case $i \neq j$. Let $f_{ij}^{(n)}$ denote the probability that, starting from state i with $X_0 = i$, the first return to state j is at the nth time step,

$$f_{ij}^{(n)} = P\{X_n = j, X_m \neq j, m = 1, 2, \cdots, n-1 \,|\, X_0 = i\}\,, \tag{29}$$

where $i \neq j$ and $n \geq 1$. The probabilities $f_{ij}^{(n)}$ are known as *first passage time probabilities.*

Also for this case,

- $$0 \leq \sum_{n=0}^{\infty} f_{ij}^{(n)} \leq 1$$

- If
$$\sum_{n=0}^{\infty} f_{ij}^{(n)} = 1$$
then the set $\{f_{ij}^{(n)}\}_{n=0}^{\infty}$ defines a probability distribution for a random variable T_{ij}, which denotes the *first passage time* from state i to state j.

- If
$$f_{ij} = \sum_{n=0}^{\infty} f_{ij}^{(n)} < 1$$
then the probability of never reaching state j from state i is $1 - f_{ij}$.

If $X_0 = i$, then the *mean first passage time* to state j is denoted $\mu_{ij} = E(T_{ij})$ and defined as

$$\mu_{ij} = \sum_{n=1}^{\infty} n\, f_{ij}^{(n)} \,, \qquad i \neq j \,. \tag{30}$$

If $f_{ij} < 1$, then the mean first passage time is infinite.

By an argument analogous to that which lead to (26), we have

$$P_{ij}^{n} = \sum_{k=0}^{n} f_{ij}^{k}\, P_{jj}^{n-k} \,, \quad i \neq j,\ n \geq 0 \,, \tag{31}$$

where f_{ij}^{k} is the probability that the first passage from state i to state j occurs at the kth transition. Again, we define $f_{ij}^{0} = 0$ for all i and j.

Various classes and properties of a Markov chain can be illustrated using a *directed graph* or *digraph*, as is shown in Fig. 5. A directed graph with N nodes (or states) constructed from a transition probability matrix P is said to be *strongly connected* if there exists a series of directed paths from i to j (with $i \leftrightarrow j$) for every $i, j \in \{0, 1, 2, \cdots, N\}$. In relation to irreducibility, a transition probability matrix P of a finite Markov chain is said to be irreducible if its directed graph is strongly connected. Alternately, a transition probability matrix P of a finite Markov chain is said to be reducible if its directed graph is not strongly connected [1].

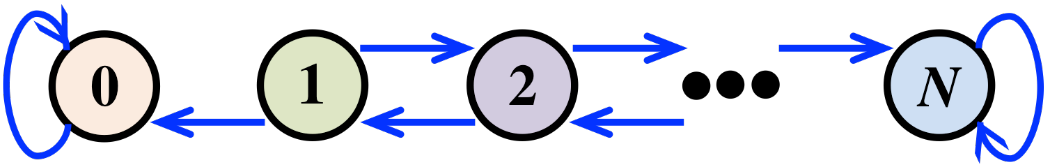

Figure 5: Directed graph of a Markov chain having states $\{0, 1, \cdots, N\}$. The Markov chain is reducible and has three communication classes: $\{0\}$, $\{1, 2, \cdots, N-1\}$, and $\{N\}$. The states $\{0\}$ and $\{N\}$ are closed and absorbing (recurrent), but the remaining states $\{1, 2, \cdots, N-1\}$ are transient and not closed.

Various classes and properties of a Markov chain can also be illustrated using the transition probability matrix,

$$P = \begin{bmatrix} P_{00} & P_{01} & 0 & 0 & 0 \\ P_{10} & P_{11} & 0 & 0 & 0 \\ 0 & 0 & P_{22} & P_{23} & P_{24} \\ 0 & 0 & P_{32} & P_{33} & P_{34} \\ 0 & 0 & P_{42} & P_{43} & P_{44} \end{bmatrix},$$

where all $P_{ij} > 0$ are nonnegative. This Markov chain clearly divides into two classes composed of states $\{0, 1\}$ and states $\{2, 3, 4\}$. Both classes are closed and transient. The Markov chain is reducible.

Example 3.7

This example is taken from **Example 4.11 in** [4]**:**
Consider the Markov chain consisting of the three states 0, 1, 2 and having transition probability matrix

$$P = \begin{bmatrix} P_{00} & P_{01} & P_{02} \\ P_{10} & P_{11} & P_{12} \\ P_{20} & P_{21} & P_{22} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{3} & \frac{2}{3} \end{bmatrix}$$

We observe only nonzero elements of the matrix. Here, we investigate the relationship between states of this Markov chain as follows:

- $0 \to 1$ with probability $P_{01} = \frac{1}{2}$ and $1 \to 0$ with probability $P_{10} = \frac{1}{2}$. Since these states 0 and 1 communicate, then $0 \leftrightarrow 1$.

- $1 \rightarrow 2$ with probability $P_{12} = \frac{1}{4}$ and $2 \rightarrow 1$ with probability $P_{21} = \frac{1}{3}$. States 1 and 2 communicate, then $1 \leftrightarrow 2$.
- Transitivity occurs, since $0 \leftrightarrow 1$, $1 \leftrightarrow 2$ which implies $0 \leftrightarrow 2$.

Since all states communicate with each other, they are in the same class $\{0, 1, 2\}$. Hence, this Markov chain is irreducible.

The probability to go from state 0 to state 2 is given by (23), thus

$$P_{02}^{(2)} = P_{01}\, P_{12} = \frac{1}{2} \cdot \frac{1}{4} = \frac{1}{8}\,,$$

and the probability to go from state 2 to state 0 is

$$P_{20}^{(2)} = P_{21}\, P_{10} = \frac{1}{3} \cdot \frac{1}{2} = \frac{1}{6}\,.$$

The directed graph of this Markov process is shown in Fig. 6. The Markov chain is strongly connected.

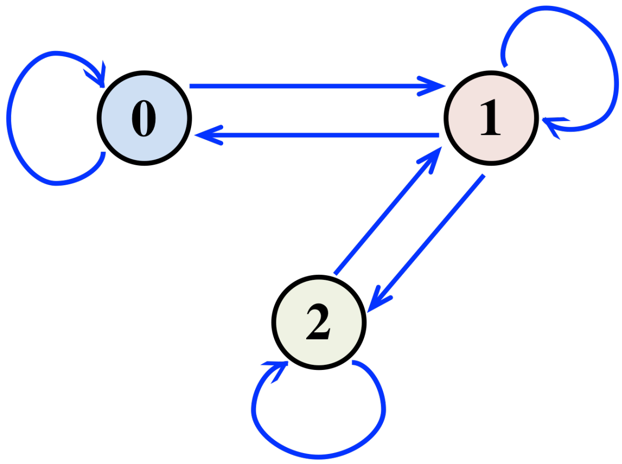

Figure 6: Directed graph of a Markov chain for Example 3.7.

Example 3.8

This example is taken from **Example 4.12 in** [4]**:**
Consider a Markov chain consisting of the four states 0, 1, 2, 3 and having transition

probability matrix

$$P = \begin{bmatrix} P_{00} & P_{01} & P_{02} & P_{03} \\ P_{10} & P_{11} & P_{12} & P_{13} \\ P_{20} & P_{21} & P_{22} & P_{23} \\ P_{30} & P_{31} & P_{32} & P_{33} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

We observe only nonzero elements of the matrix. First, we notice that state 3 only communicates with itself, that is $P_{33} = 1$, and there is no other state that is accessible from it. Hence, state 3 forms a single communication class by itself, $\{3\}$. Then, we are left with states 0, 1, 2 to investigate:

(1) From state 0 to state 1, the probability is $P_{01} = \frac{1}{2}$, or $0 \to 1$. From state 1 to state 0, the probability is $P_{10} = \frac{1}{2}$, or $1 \to 0$. Hence states 0 and 1 communicate, or $0 \leftrightarrow 1$. State 0 and state 1 are in the same class, $\{0, 1\}$.

(2) From state 0 to state 2, the probability is $P_{02} = 0$, or $0 \nrightarrow 2$. However, from state 2 to state 0, the probability is $P_{20} = \frac{1}{4}$, or $2 \to 0$. States 0 and 2 do not communicate.

(3) From state 1 to state 2, the probability is $P_{12} = 0$, or $1 \nrightarrow 2$. However, from state 2 to state 1, the probability is $P_{21} = \frac{1}{4}$, or $2 \to 1$. States 1 and 2 do not communicate.

(4) From items (2) and (3) above, it is impossible to return to state 2 after having left it. This state 2 forms a single communication class $\{2\}$

Therefore, the classes of this Markov chain are $\{0, 1\}$, $\{2\}$, and $\{3\}$, and this Markov chain is reducible.

The transition diagram (or directed graph) of this Markov process is shown in Fig. 7.

Example 3.9

This example is taken from **Example 2.8 in [1]:**
Suppose the transition matrix of a two-state Markov chain is

$$\mathbf{P} = \begin{bmatrix} P_{00} & P_{01} \\ P_{10} & P_{11} \end{bmatrix},$$

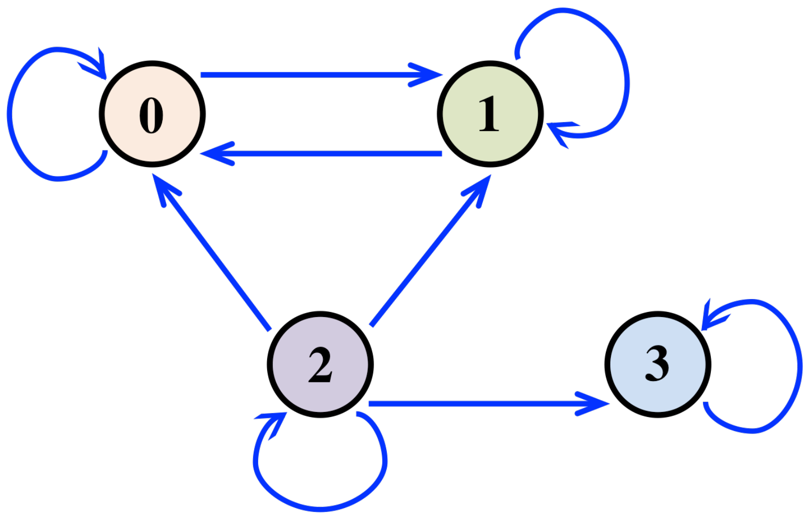

Figure 7: A directed graph of a Markov chain for Example 3.8.

where $0 < P_{ii} < 1$ for $i = 0, 1$. All of the elements of matrix $\mathbf{P}$ are positive, $P_{ij} > 0$, for $i, j = 0, 1$.

From equation (29) and by (23) and $f_{ii}^{(1)} = P_{ii}$, we show that,

$$f_{00}^{(1)} = P\{X_1 = 0 \,|\, X_0 = 0\} = P_{00}^{(1-0)} = P_{00}^{(1)} = P_{00}$$

$$\begin{aligned}
f_{00}^{(2)} &= P\{X_2 = 0, X_1 = 1 \,|\, X_0 = 0\} \\
&= P\{X_2 = 0 \,|\, X_1 = 1\}\, P\{X_1 = 1 \,|\, X_0 = 0\} \\
&= P_{10}^{(2-1)}\, P_{01}^{(1-0)} \\
&= P_{01}\, P_{10}
\end{aligned}$$

$$\begin{aligned}
f_{00}^{(3)} &= P\{X_3 = 0, X_2 = 1, X_1 = 1 \,|\, X_0 = 0\} \\
&= P\{X_3 = 0, X_2 = 1 \,|\, X_1 = 1\}\, P\{X_1 = 1 \,|\, X_0 = 0\} \\
&= P\{X_3 = 0 \,|\, X_2 = 1\}\, P\{X_2 = 1 \,|\, X_1 = 1\}\, P\{X_1 = 1 \,|\, X_0 = 0\} \\
&= P_{10}^{(3-2)}\, P_{11}^{(2-1)}\, P_{01}^{(1-0)} \\
&= P_{01}\, P_{11}\, P_{10}
\end{aligned}$$

From the last result, if

$$n = 4 \quad \longrightarrow \quad f_{00}^{(4)} = P_{01}\, P_{11}\, P_{11}\, P_{10} = P_{01}\, P_{11}^2\, P_{10}$$

$$n = 5 \quad \longrightarrow \quad f_{00}^{(5)} = P_{01}\, P_{11}\, P_{11}\, P_{11}\, P_{10} = P_{01}\, P_{11}^3\, P_{10}$$

In general,

$$f_{00}^{(n)} = P_{01}\, P_{11}^{(n-2)}\, P_{10}\,, \qquad \text{for } \ n \geq 3\,.$$

Because $P_{11} < 1$, then,

$$\sum_{n=1}^{\infty} f_{00}^{(n)} = P_{00} + P_{01}\, P_{10} \sum_{n=0}^{\infty} P_{11}^{n}\,.$$

Due to geometric progression of $\sum_{n=0}^{\infty} P_{11}^{n}$, where the sum of infinite terms is

$$\sum_{n=0}^{\infty} P_{11}^{n} = \frac{1}{1 - P_{11}}\,,$$

then,

$$\sum_{n=1}^{\infty} f_{00}^{(n)} = P_{00} + \frac{P_{01}\, P_{10}}{1 - P_{11}}\,.$$

From the definition of a stochastic matrix, $P_{00}+P_{01} = 1$ and $P_{10}+P_{11} = 1$ or $P_{10} = 1-P_{11}$, it follows that

$$\begin{aligned} \sum_{n=1}^{\infty} f_{00}^{(n)} &= P_{00} + \frac{P_{01}\, P_{10}}{P_{10}} \\ &= P_{00} + P_{01} \\ &= 1\,. \end{aligned}$$

This implies that state 0 is recurrent. Similarly, it can be shown that state 1 is also recurrent, by the mean recurrence times which are calculated using (28),

$$\begin{aligned} \mu_{00} &= \sum_{n=1}^{\infty} n\, f_{00}^{(n)} \\ &= 1 \cdot f_{00}^{(1)} + 2 \cdot f_{00}^{(2)} + 3 \cdot f_{00}^{(3)} + 4 \cdot f_{00}^{(4)} + \cdots \\ &= P_{00} + 2 \cdot P_{01} \cdot P_{10} + 3 \cdot P_{01} \cdot P_{11} \cdot P_{10} + 4 \cdot P_{01} \cdot P_{11}^{2} \cdot P_{10} + \cdots \\ &= P_{00} + P_{01}\, P_{10} + \sum_{n=0}^{\infty} (n+2)\, P_{11}^{n} < \infty\,. \end{aligned}$$

Thus, both states 0 and 1 are positive (non-null) recurrent.

3 Random Walk Models

In this lecture, we use the terminology "random walk" for discrete-time Markov chain models.

Random walks serve as reasonable discrete approximations to many phenomena in physics, such as in describing the motion of diffusing particles. In discussing random walks, it is helpful to speak about the state of the system as the position of a moving particle. If a particle is subjected to collisions and random impulses, then its position fluctuates randomly, although the particle describes a continuous path. If the future position (or the probability distribution) of the particle depends only on the present position, then the process $\{X_n\}$ where X_n is the position at time n, is Markovian. A discrete approximation to such a continuous motion corresponds to a random walk.

Normally, random walk models are classified into *restricted* and *unrestricted* random walks:

- A restricted random walk is a random walk model with at least one boundary, so that either the state space of the chain is finite, $\{0, 1, 2, \cdots, N\}$ with boundaries at 0 and N, or semi-finite, $\{0, 1, 2, \cdots\}$ with one boundary at 0.
- An unrestricted random walk is a random walk model without boundaries.

3.1 One Dimensional Random Walks

A one-dimensional random walk is a Markov chain whose state space is a finite or infinite subset of integers, in which, the particle, if it is in state i, can in a single transition either stay in i or move to one of the adjacent states $i-1$ or $i+1$. If the state space is taken as the nonnegative integers, the probability of the particle moving to the right is given by,

$$P\{X_{n+1} = i+1 \,|\, X_n = i\} = P_{i,i+1} = p_i \,,$$

the probability of the particle moving to the left is given by,

$$P\{X_{n+1} = i-1 \,|\, X_n = i\} = P_{i,i-1} = q_i \,,$$

and the probability of the particle staying in state i is given by,

$$P\{X_{n+1} = i \,|\, X_n = i\} = P_{i,i} = r_i \,,$$

whereas everything else is zero. The transition probability matrix of the random walk has the form

$$\mathbf{P} = \begin{bmatrix} r_0 & p_0 & 0 & 0 & \cdots & 0 & 0 \\ q_1 & r_1 & p_1 & 0 & \cdots & 0 & 0 \\ 0 & q_2 & r_2 & p_2 & \cdots & 0 & 0 \\ 0 & 0 & q_3 & r_3 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & 0 & q_i & r_i & p_i \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \tag{32}$$

where $p_i > 0$, $q_i > 0$, $r \geq 0$, and $q_i + r_i + p_i = 1$ for $i = 1, 2, 3, \cdots$ and $p_0 \geq 0$, $r_0 \geq 0$, $r_0 + p_0 = 1$.

The nature of state 0 determines different processes and is classified as follows:

(a) If $r_0 = 0$ and $p_0 = 1$, then state 0 acts like a reflecting boundary. Whenever the particle reaches state 0, the next transition automatically returns it to state 1. A directed graph of this process is shown in Fig. 8(a).

(b) If $r_0 = 1$ and $p_0 = 0$, state 0 acts as an absorbing boundary. Once the particle reaches state 0, it remains in that state forever. Directed graph of this process is shown in Fig. 8(b).

(c) If $r_0 > 0$ and $p_0 > 0$, state 0 is a partially reflecting boundary. Directed graph of this process is shown in Fig. 8(c).

(d) When the random walk is restricted to a finite number of states $\mathcal{C} = \{1, 2, \cdots, N\}$, then both states 0 and N independently and in any combination may be reflecting, absorbing, or partially reflecting boundaries.

The Ehrenfest model is an example of a random walk on a finite set of states with reflecting boundary states. It is a classical mathematical model of diffusion through a membrane. The random walk is restricted to the states $i = -N, -N+1, \cdots, -1, 0, 1, \cdots, N$ with a transition probability matrix given by,

$$P_{ij} = \begin{cases} \dfrac{N-i}{2N}\,, & \text{if } \; j = i+1 \\[2ex] \dfrac{N+i}{2N}\,, & \text{if } \; j = i-1 \\[2ex] 0\,, & \text{otherwise} \end{cases}$$

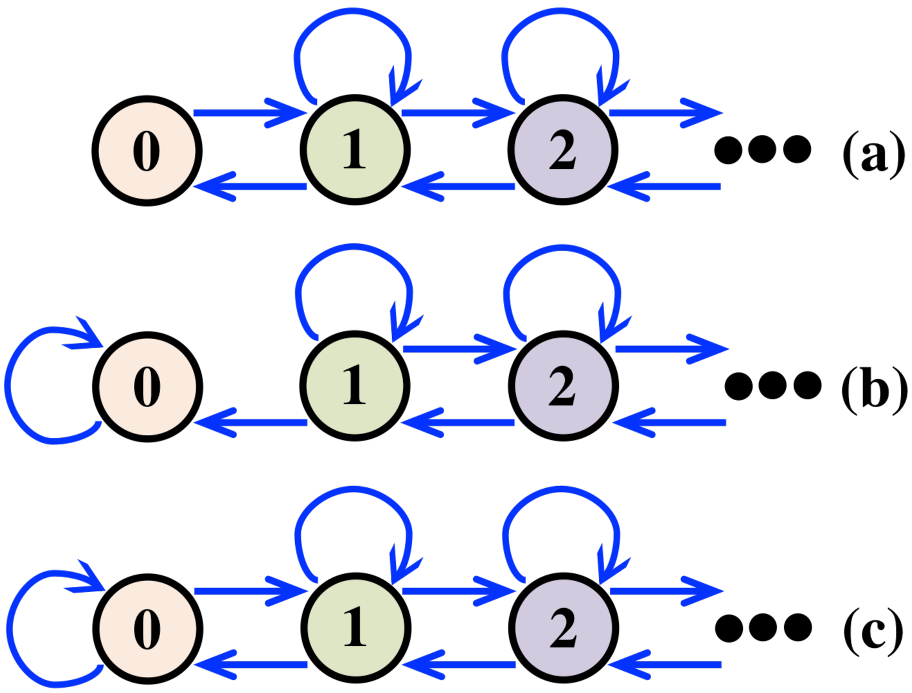

Figure 8: Directed graphs of various processes of 1D random walks: (a) state 0 acts like a reflecting boundary, (b) state 0 is an absorbing boundary, and (c) state 0 is a partially reflecting boundary.

or,

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & & & & & & \\ \frac{1}{2N} & 0 & \frac{2N-1}{2N} & & & & & & \\ 0 & \ddots & \ddots & \ddots & & & & & \\ & & \frac{N-1}{2N} & 0 & \frac{N+1}{2N} & & & & \\ & & & \frac{1}{2} & 0 & \frac{1}{2} & & & \\ & & & & \frac{N+1}{2N} & 0 & \frac{N-1}{2N} & & \\ & & & & & \ddots & \ddots & \ddots & \\ & & & & & & \frac{2N-1}{2N} & 0 & \frac{1}{2N} \\ & & & & & & 0 & 1 & 0 \end{bmatrix}$$

The directed graph for the Ehrenfest model is shown in Fig. 9.

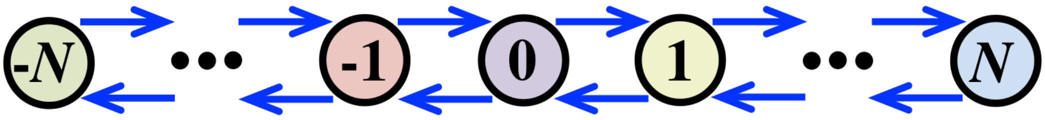

Figure 9: Directed graph of the Ehrenfest model, an unrestricted random walk on a finite set of states, where boundaries are reflecting.

In an infinite-dimensional random walk, or unrestricted random walk, the states are integers $0, \pm 1, \pm 2, \cdots$. Let $p > 0$ be the probability of moving to the right and $q > 0$ be the probability of moving to the left, where $p + q = 1$. There are no absorbing boundaries, with a transition probability matrix is given by,

$$P_{ij} = \begin{cases} p & \text{if } j = i + 1 \\ \\ q & \text{if } j = i - 1 \end{cases}$$

for $i \in \{0, \pm 1, \pm 2, \cdots\}$. From the directed graph in Fig. 10, the Markov chain is irreducible, Every state in the system communicates with every other state. The set of states forms a closed set. The transition probability matrix $\mathbf{P}$ is infinite dimensional.

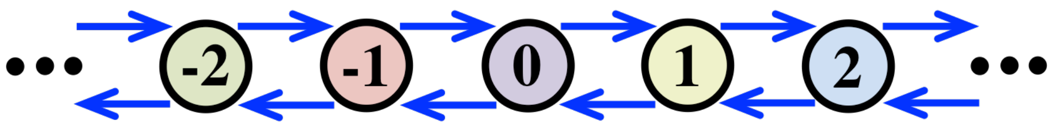

Figure 10: Directed graph of an unrestricted random walk on an infinite set of states.

3.2 Symmetric Random Walks

Consider a Markov chain whose state space consists of the integers $i = 0, \pm 1, \pm 2, \cdots$, and the transition probabilities are given by

$$\begin{aligned} P_{i,i+1} &= p \\ P_{i,i-1} &= q \end{aligned}$$

where $0 < p < 1$, $0 < q < 1$, and $p + q = 1$. On each transition, the process either moves one step to the right (with probability p) or one step to the left (with probability q). This process is a one-dimensional unrestricted random walk, as shown by example in Fig. 10. Since all states clearly communicate, they are either all transient or all recurrent. Let us consider state 0 or the origin. If the origin is recurrent, then all states are recurrent because the chain is irreducible. Notice that starting from the origin, it is impossible to return to the origin in an odd number of steps,

$$P_{00}^{(2n-1)} = 0\,, \qquad n = 1, 2, 3, \cdots$$

On the other hand, in $2n$ steps, there are a total of n steps to the right and a total of n steps to the left. Because each step results in movement to the right with probability p and movement to the left with probability $q = 1 - p$, the desired probability is thus the binomial probability

$$P_{00}^{(2n)} = \binom{2n}{n} p^n (1-p)^n = \frac{(2n)!}{n!n!}\,(p(1-p))^n\;, \quad n = 1, 2, 3, \cdots$$

An asymptotic formula to approximate $n!$, known as Stirling's formula, given by

$$n! \sim n^{n+1/2}\,e^{-n}\,\sqrt{2\pi}\,,$$

is used to verify the recurrence. The notation $a_n \sim b_n$ means that a_n and b_n grow at the same rate as $n \to \infty$:

$$\lim_{n\to\infty} \frac{a_n}{b_n} = 1$$

Applying Stirling's formula yields the following approximation:

$$\begin{aligned} P_{00}^{(2n)} &= \frac{(2n)!}{n!n!}\,(p(1-p))^n \\ &\sim \frac{\sqrt{4\pi n}\,(2n)^{2n}\,e^{-2n}}{2\pi n^{2n+1}\,e^{-2n}}(p(1-p))^n \\ &= \frac{(4p(1-p))^n}{\sqrt{\pi n}} \end{aligned}$$

It is now easy to verify, for positive a_n, b_n, that if $a_n \sim b_n$, then $\sum\limits_n a_n < \infty$ if and only if $\sum\limits_n b_n < \infty$. Therefore, $\sum\limits_{n=1}^{\infty} P_{00}^{(2n)}$ will converge if and only if

$$\sum_{n=1}^{\infty} \frac{(4p(1-p))^n}{\sqrt{\pi n}}$$

converges. However, the expression $4p(1-p)$ has a maximum at $p = \frac{1}{2}$. If $p = \frac{1}{2}$, then $4p(1-p) = 1$ and if $p \neq \frac{1}{2}$, then $4p(1-p) < 1$. Thus,

- if $p \neq \frac{1}{2}$, then

$$\sum_{n=1}^{\infty} P_{00}^{(2n)} = \sum_{n=1}^{\infty} \frac{(4p(1-p))^n}{\sqrt{\pi n}} = \frac{1}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(4p(1-p))^n}{\sqrt{n}} < \infty$$

- if $p = \frac{1}{2}$, then the series

$$\sum_{n=1}^{\infty} P_{00}^{(2n)} = \sum_{n=1}^{\infty} \frac{1}{\sqrt{\pi n}} = \frac{1}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}},$$

behaves like a p-series that diverges. To see why it diverges, notice that when n is a square number, say $n = k^2$, the nth term equals $\frac{1}{k}$ (see the terms highlighted in purple),

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} = \underbrace{1}_{k=1} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \underbrace{\frac{1}{2}}_{k=2} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{7}} + \frac{1}{\sqrt{8}} + \underbrace{\frac{1}{3}}_{k=3} + \cdots$$

The $\frac{1}{k}$ terms are harmonic series that is divergent. Thus, this p-series includes every term in harmonic series and many other terms. Because the harmonic series is divergent, this p-series is also divergent.

Hence, the series $\sum_{n=1}^{\infty} P_{00}^{(2n)} = \infty$ diverges if and only if $p = \frac{1}{2}$. Thus, the chain is recurrent if $p = \frac{1}{2}$, which is called a *symmetric random walk* or *unbiased random walk*. When $p \neq \frac{1}{2}$, then all states are transient and the chain/random walk is transient, or also called a *biased random walk*. In a transient chain, there is a positive probability that an object starting from the origin will never return to the origin [4, 1].

An example of the transition probability matrix of a symmetric random walk with reflecting boundary on $\{0, \cdots, 4\}$:

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

An example of the transition probability matrix of a symmetric random walk with absorbing boundary on $\{0, \cdots, 4\}$:

$$\mathbf{P} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

3.3 Unrestricted Random Walk in Higher Dimensions

One-dimensional random walk models can be extended to two and three dimensions. For higher dimension random walks, it is assumed that the probability of moving in any one direction is,

- For two dimensions, the probability is $\frac{1}{4}$ of moving in any of the four directions: up, down, right, or left.
- For three dimensions, the probability is $\frac{1}{6}$ of moving in any of the six directions: up, down, right, left, forward, or backward.

In general, the classical symmetric random walk in m dimensions follows the following formulation. The state space is identified with the set of all integral lattice points in E^m (Euclidean m space), where, a state is an m-tuple $\mathbf{k} = (k_1, k_2, \cdots, k_m)$ of integers. The transition probability matrix is defined by,

$$\mathbf{P} = \begin{cases} \dfrac{1}{2m} & \text{if } \displaystyle\sum_{i=1}^{m} |\, l_i - k_i \,| = 1 \\ \\ 0 & \text{otherwise}\,. \end{cases} \tag{33}$$

The difference between random walks in one, two, and three dimensions is that,

- ▷ One dimension: the Markov chain is null recurrent if and only if $p = \frac{1}{2} = q$, where p is the probability of moving to the right and q is the probability of moving to the left.
- ▷ Two dimension: the Markov chain is null recurrent.
- ▷ Three dimension: the Markov chain is transient.

The Markov chain represented by an unrestricted random walk is irreducible and periodic of period 2. Let 0 denote the origin and $P_{00}^{(n)}$ denote the probability of returning to the origin after n steps. Note that $P_{00}^{(2n)} > 0$, but $P_{00}^{(2n+1)} = 0$ for $n = 0, 1, 2, \cdots$. If the walk starts at the origin, it must take an even number of steps to return to the origin.

3.3.1 Random Walk in Two Dimensions

In two dimensional random walk, the process at each transition would either take one step to the right, left, up, or down, each having probability $\frac{1}{4}$. That is, the state is the pair of integers (i, j) and the transition probabilities are given by [4]

$$P_{(i,j),(i+1,j)} = P_{(i,j),(i-1,j)} = P_{(i,j),(i,j+1)} = P_{(i,j),(i,j-1)} = \frac{1}{4} \tag{34}$$

Consider $P_{00}^{(2n)}$. For a path length of $2n$, after $2n$ steps, the chain will be back in its original location if for some k, $0 \leq k \leq n$, the $2n$ steps consist of k steps are taken to the left, k steps to the right, $n-k$ steps in the upward direction, and $n-k$ steps downward, making $k+k+n-k+n-k=2n$. There are

$$\sum_{k=0}^{n} \frac{(2n)!}{k!k!(n-k)!(n-k)!}$$

different paths of length $2n$ that begin and end at the origin. Each of these paths is equally likely and has a probability of occurring equal to $(1/4)^{2n}$. That is,

$$\begin{aligned} P_{00}^{(2n)} &= \sum_{k=0}^{n} \frac{(2n)!}{k!k!(n-k)!(n-k)!} \left(\frac{1}{4}\right)^{2n} \\ &= \sum_{k=0}^{n} \frac{(2n)!}{n!n!} \frac{n!}{(n-k)!k!} \frac{n!}{(n-k)!k!} \left(\frac{1}{4}\right)^{2n} \end{aligned}$$

Since,

$$\frac{n!}{(n-k)!k!} = \binom{n}{k},$$

also,

$$\frac{n!}{(n-k)!k!} = \binom{n}{n-k},$$

then

$$P_{00}^{(2n)} = \frac{(2n)!}{n!n!} \left(\frac{1}{4}\right)^{2n} \sum_{k=0}^{n} \binom{n}{k} \binom{n}{n-k}.$$

Due to the combinatorial identity, where

$$\binom{2n}{n} = \sum_{k=0}^{n} \binom{n}{k} \binom{n}{n-k},$$

and due to

$$\binom{2n}{n} = \frac{(2n)!}{(2n-n)!n!} = \frac{(2n)!}{n!n!},$$

hence $P_{0}^{(2n)}$ can be simplified to

$$P_{00}^{(2n)} = \binom{2n}{n} \binom{2n}{n} \left(\frac{1}{4}\right)^{2n}.$$

Now,

$$\begin{aligned} \binom{2n}{n} &= \frac{(2n)!}{n!n!} \\ &\sim \frac{(2n)^{2n+1/2}\, e^{-2n}\, \sqrt{2\pi}}{n^{2n+1}\, e^{-2n}\, (2\pi)} \quad \text{by Stirling's approximation} \\ &= \frac{4^n}{\sqrt{\pi n}}, \end{aligned}$$

thus

$$P_{00}^{(2n)} = \left(\frac{4^n}{\sqrt{\pi n}}\right)^2 \left(\frac{1}{4^{2n}}\right) = \frac{1}{\pi n},$$

which shows that $\sum_n P_{00}^{(2n)} = \infty$ (diverges) and thus, all states are recurrent.

3.3.2 Random Walk in Three Dimensions

Despite the symmetric random walks in one and two dimensions are both recurrent, in three and higher dimensions, symmetric random walks turn out to be transient.

In three dimensions, in a path of length $2n$ beginning and ending at the origin, the process at each transition consists of: if k steps are taken to the right, then k steps must be taken to the left; if j steps are taken upward, then j steps must be taken downward; if $n-k-j$ steps are taken forward, then $n-k-j$ steps must be taken backward, together making $k+k+j+j+n-k-j+n-k-j = 2n$. There are total

$$\sum_{j+k\le n} \frac{(2n)!}{(k!)^2(j!)^2((n-k-j)!)^2}$$

different paths of length $2n$ that begin and end at the origin. The sum is over all of j and k, where $j+k \le n$.

It will be shown that the $\sum P_{00}^{(2n)}$ converges and the origin is a transient state, hence the Markov chain is transient. The verification of this is in [1].

Example 3.10: Restricted Random Walk Model with Absorbing Boundaries

This example is taken from **Example 2.3 in [1]:**
A random walk model considers the state of a system as the position of a moving "particle".

The state space of a random walk model is the set $\{0, 1, 2, \cdots, N\}$. The probability of the particle moving to the right is given by

$$P_{i,i+1} = p\,, \qquad p > 0$$

the probability of moving to the left is given by

$$P_{i,i-1} = q\,, \qquad q > 0$$

where for both probabilities, $i = 1, 2, \cdots, N-1$ and $p + q = 1$. In addition, $P_{00} = 1$ and $P_{NN} = 1$, which are referred to as absorbing boundaries, and everywhere else is zero. The corresponding transition matrix is

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ q & 0 & p & 0 & \cdots & 0 & 0 & 0 \\ 0 & q & 0 & p & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & & & & \cdots & q & 0 & p \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{bmatrix}$$

The Markov chain has three communication classes: $\{0\}$, $\{1, 2, \cdots, N-1\}$, and $\{N\}$. The Markov chain is reducible. The sets $\{0\}$ and $\{N\}$ are closed, but the set $\{1, 2, \cdots, N-1\}$ is not closed. Also, states 0 and N are absorbing; whereas the remaining states are transient. The directed graph for this Markov chain is exactly the same as that shown in Fig. 5. This Markov chains is an example where it is possible to reach the first class $\{0\}$ or third class $\{N\}$ from the second class $\{1, 2, \cdots, N-1\}$, but it is not possible to return to the second class from either the first or the third class.

Example 3.11: Unrestricted Random Walk Model

This example is taken from **Example 2.4 in [1]:**
In an infinite-dimensional random walk, or unrestricted random walk, the states are the integers $0, \pm 1, \pm 2, \cdots$. Let $p > 0$ be the probability of moving to the right and $q > 0$ be the probability of moving to the left, with $p + q = 1$. There are no absorbing boundaries, $P_{i,i+1} = q$ and $P_{i,i-1} = p$ for $i \in \{0, \pm 1, \pm 2, \cdots\}$. The directed graph for this unrestricted random walk model is similar to that shown in Fig. 10. From the directed graph, we observe that the Markov chain is irreducible. Every state in the system communicates with every other state. The set of states forms a closed set. The transition probability matrix is infinite dimensional.

4 Python Implementation

All code implemented here use Python 3.6. The Python code of the following examples are available on the course website.

Python Code 1

Let us apply the Example 3.5 in Section 2 (n-Step Transition Probabilities) by first importing the NumPy library we are going to use here,

```
import numpy as np
```

There are four states of the Markov chain. Hence the state space is defined as follows,

```
states = ["0", "1", "2", "3"]
```

Following the transition probability matrix of the four-state Markov chain, we define the possible sequence of events in a matrix as follows,

```
possibleEvents = [["00", "01", "02", "03"], ["10", "11", "12", "13"],
                  ["20", "21", "22", "23"], ["30", "31", "32", "33"]]
```

and the values of the transition probability matrix

```
transitionMatrix = [[0.7, 0.0, 0.3, 0.0], [0.5, 0.0, 0.5, 0.0],
                    [0.0, 0.4, 0.0, 0.6], [0.0, 0.2, 0.0, 0.8]]
```

The possible states and probability value for the weather forecast problem are calculated in the following function,

```
def weather_forecast(days, initialWeather):
    weatherToday = initialWeather
    weatherList = [weatherToday]
    k = 0
    prob = 1.0
    while k < days:
        if weatherToday == "0":
            event = np.random.choice(possibleEvents[0], replace=True, p=
                                      transitionMatrix[0])
            if event == "00":
                prob *= transitionMatrix[0][0]
            elif event == "01":
                prob *= transitionMatrix[0][1]
                weatherToday = "1"
            elif event == "02":
                prob *= transitionMatrix[0][2]
```

```
                weatherToday = "2"
            else:
                prob *= transitionMatrix[0][3]
                weatherToday = "3"
            weatherList.append(weatherToday)
        elif weatherToday == "1":
            event = np.random.choice(possibleEvents[1], replace=True, p=
                                                 transitionMatrix[1])
            if event == "11":
                prob *= transitionMatrix[1][1]
            elif event == "10":
                prob *= transitionMatrix[1][0]
                weatherToday = "0"
            elif event == "12":
                prob *= transitionMatrix[1][2]
                weatherToday = "2"
            else:
                prob *= transitionMatrix[1][3]
                weatherToday = "3"
            weatherList.append(weatherToday)
        elif weatherToday == "2":
            event = np.random.choice(possibleEvents[2], replace=True, p=
                                                 transitionMatrix[2])
            if event == "22":
                prob *= transitionMatrix[2][2]
            elif event == "20":
                prob *= transitionMatrix[2][0]
                weatherToday = "0"
            elif event == "21":
                prob *= transitionMatrix[2][1]
                weatherToday = "1"
            else:
                prob *= transitionMatrix[2][3]
                weatherToday = "3"
            weatherList.append(weatherToday)
        elif weatherToday == "3":
            event = np.random.choice(possibleEvents[3], replace=True, p=
                                                 transitionMatrix[3])
            if event == "33":
                prob *= transitionMatrix[3][3]
            elif event == "30":
                prob *= transitionMatrix[3][0]
                weatherToday = "0"
            elif event == "31":
                prob *= transitionMatrix[3][1]
                weatherToday = "1"
            else:
                prob *= transitionMatrix[3][2]
                weatherToday = "2"
            weatherList.append(weatherToday)
```

```
        k += 1

    return [weatherList, prob]
```

We use the `numpy.random.choice()` to generate a random sample from the set of possible events. The function takes two input arguments: `days` and `initialWeather` and returns a list that consists of possible weather states and a probability value.

As an example, we set the following input arguments,

```
days = 2
init = states[0]
```

for the function

```
[weatherStates, probVal] = weather_forecast(days, init)
```

In the initial values, we set "0" as the initial state and calculate the probability after 2 days. If we run the code until we get "0" as the end state, we get a probability 0.4899, which is the probability P^2_{00} in the Example 3.5. Likewise, if we run the code until we get "1" as the end state, we get a probability 0.12, which the probability P^2_{01}.

The Python code for this example is named `mc_4states.py`, available on the course website.

Python Code 2

Here we implement a simple one-dimensional random walk model in Python. In the random walk model, the states are positions and are denoted by the variable x, that is $x = 0, 1, 2, \cdots$ and time is denoted as n. It is assumed that p is the probability of moving to the right, x to $x + 1$, and q is the probability of moving to the left, x to $x - 1$, that is $p + q = 1$.

First we import the "random" library,

```
import random
```

which we use to generate a sample of random floating point number in the range $[0.0, 1.0)$.

```
prob = random.random()
```

If the sample generates a floating point number bigger than 0.5, the particle moves one step to the right. On the hand, if the generated random number is less than 0.5, the particle moves one step to the left.

```
if prob > 0.5:
    x = x + 1
```

```
elif prob < 0.5:
    x = x - 1
```

We set 0 as the initial position, and initialize it by defining $x = 0$. We would also want to keep track the movement of the particle each time. This is done by storing the position each time in the list `c`. The function to simulate a one-dimensional random walk is as follows:

```
def random_walk(n):
    x = 0
    c = [x]
    for i in range(n):
        prob = random.random()
        if prob > 0.5:
            x = x + 1
        elif prob < 0.5:
            x = x - 1
        c.append(x)
    return c
```

The Python code for this example is named `randomwalk1d.py`, and available on the course website.

The above example of simulating a one-dimensional random walk uses the `for` loop, in which the calculation is iterated over the range $(0, n)$. Another way to simulate the random walk is by by replacing the `for` loop with higher level "vectorized" commands, as follows,

```
import numpy as np

steps = 2*np.random.randint(0, 2, n) - 1
steps[0] = 0

movement = np.cumsum(steps)
```

The variable `steps` produces a randomly generated array of 1s and -1s of length n. If it is 1, the particle moves to the right and -1 means the particle moves to the left. We set 0 as the initial position, hence the first element of the array is taken to be zero, `steps[0] = 0`.

The Python code for this example is named `vectorized_randomwalk1d.py`, and available on the course website.

An example of the one-dimensional random walk is plotted in Fig. 11, with $n = 100$.

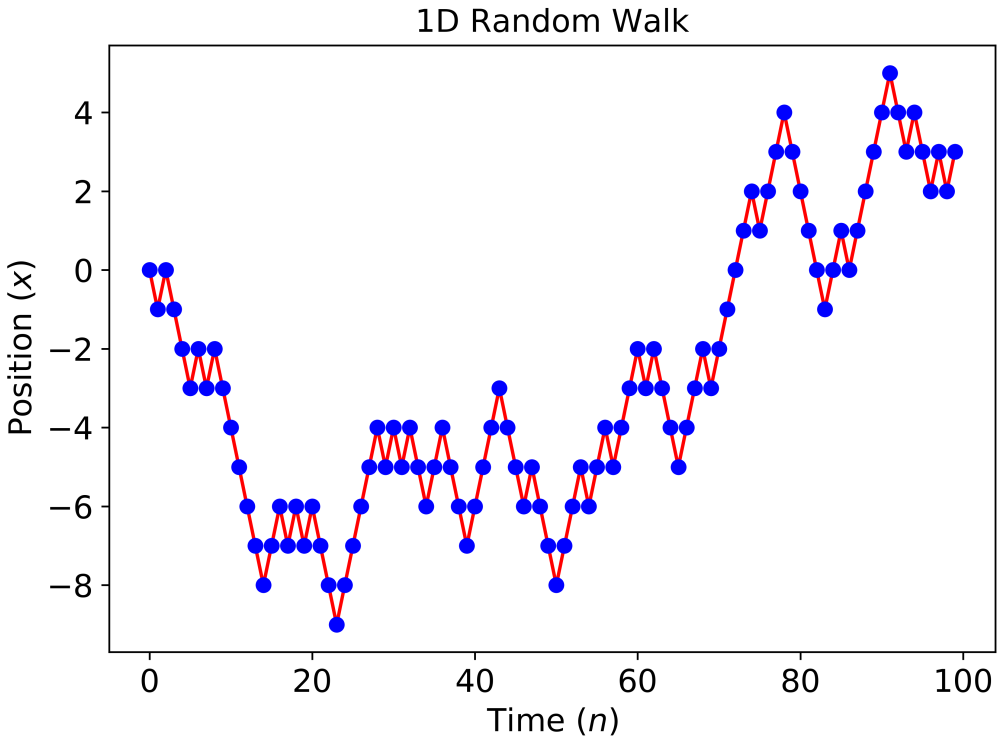

Figure 11: An example of one-dimensional random walk.

References

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