

# An Introduction to Markov Chains

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## Introduction

In the year 1906, Russian mathematician Andrey Markov published his first paper introducing a probabilistic model that analyses sequences of events, which would later be designated as *Markov chains* or *Markov Processes*. His work has been extensively employed in many important fields such as Natural Language Processing (NLP), PageRank, speech recognition, robot localization, etc.

## 1 Markov Chain

A Markov chain describes a discrete-time stochastic process that consists of a finite (or infinite) set of states, which is also known as a *state space*. Initially, the process begins at any one of these states and then successively "steps" from one state to another according to some probability known as a *transition probability*. If the process is currently at state  $i$ , then we denote the probability that it transitions to state  $j$  in one step as  $p_{ij}$ .

Furthermore, consider a sequence of random variables  $\mathbf{X} = \{X_n \in S | n \in T\}$  where  $T$  is a discrete time index set. Then we say  $\mathbf{X}$  is a Markov chain if and only if, at any given time  $n$ , the conditional probability distribution for future states of the process depends only on the present state and not past states. In mathematical notation, this memoryless property can be expressed as

$$p_{ij} = P(X_{n+1} = j | X_n = i, X_{n-1}, \dots, X_0) = P(X_{n+1} = j | X_n = i)$$

This is formally known as the *Markov property* or *Markov assumption*

### 1.1 Time Homogeneity

An important assumption that we impose on Markov chains is that the conditional probability distribution of  $X_{n+1}$  given  $X_n$  is *independent* of the time  $n$ . Hence, for any state  $i, j \in S$ , and time index  $n \in T$ , the following time-invariant property holds.

$$p_{ij} = P(X_{n+1} = j | X_n = i)$$

In contrast, processes whose transition probabilities do depend on the time index  $n$  are called *time-inhomogeneous*. For our purposes, we will only focus on *time-homogeneous* processes.

## 1.2 Transition Probabilities

For a single-step transition, recall that the probability of moving from state  $i$  to  $j$  is denoted as  $p_{ij}$ . However, this notation quickly becomes strenuous if we wish to determine the evolution of the process after 2 or more steps. For that reason, we introduce a parameter  $n$  where  $p_{ij}(n)$  denotes the  $n$ -step transition probability, that is, the probability of moving from state  $i$  to  $j$  in exactly  $n$  steps.

$$p_{ij}(n) = P(X_n = j | X_0 = i)$$

For example, consider a Markov chain with state space  $S = \{s_1, s_2, s_3\}$  which starts at  $s_1$ . If we wish to determine the probability of moving to  $s_3$  in exactly 2 steps, then, by the law of total probability, we must consider every possible route from  $s_1$  to  $s_3$ .

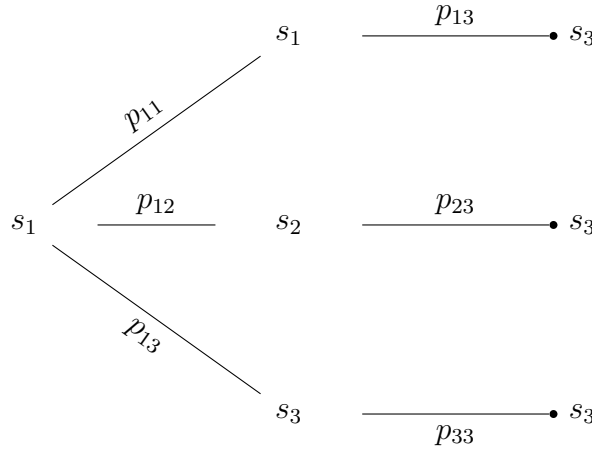


Figure 1: Probability Tree Diagram of Routes From  $s_1$  to  $s_3$

As such, the probability of moving from  $s_1$  to  $s_3$  in 2 steps is

$$p_{13}(2) = p_{11}p_{13} + p_{12}p_{23} + p_{13}p_{33} \quad (1)$$

Notice that the above equation is closely related to a dot product between two probability vectors. To make better use of this observation, we introduce some notation. Let  $m = |S|$ , then we define the *transition matrix*  $\mathbf{P} \in \mathbb{R}^{m \times m}$  where the  $(i, j)$  entry corresponds to the transition probability  $p_{ij}$ . In our example, the *transition matrix* is written as

$$\mathbf{P} = \begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{12} & p_{22} & p_{23} \\ p_{13} & p_{32} & p_{33} \end{pmatrix}$$

Notice in (1) we are dotting the first row with the third column of  $\mathbf{P}$  to obtain the probability that the process starting at  $s_1$  finishes at  $s_3$  in 2 steps. We can further generalize this observation for any 2-step transition probability.

$$\begin{aligned}
p_{ij}(2) &= P(X_2 = j | X_0 = i) \\
&= \sum_{k \in S} P(X_2 = j \cap X_1 = k | X_0 = i) \\
&= \sum_{k \in S} \frac{P(X_2 = j \cap X_1 = k \cap X_0 = i)}{P(X_0 = i)} \quad \text{Bayes' Theorem} \\
&= \sum_{k \in S} \frac{P(X_2 = j | X_1 = k \cap X_0 = i) P(X_1 = k \cap X_0 = i)}{P(X_0 = i)} \\
&= \sum_{k \in S} P(X_2 = j | X_1 = k \cap X_0 = i) P(X_1 = k | X_0 = i) \\
&= \sum_{k \in S} P(X_2 = j | X_1 = k) P(X_1 = k | X_0 = i) \quad \text{Markov Property} \\
&= \sum_{k \in S} p_{kj} p_{ik} \\
&= (\mathbf{P}^2)_{ij}
\end{aligned}$$

It follows that the second power of the transition matrix  $\mathbf{P}$  summarizes every 2-step transition probability from  $i$  to  $j$  (i.e.  $p_{ij}(2)$ ).

$$\mathbf{P}^2 = \begin{pmatrix} p_{11}(2) & p_{12}(2) & p_{13}(2) \\ p_{21}(2) & p_{22}(2) & p_{23}(2) \\ p_{31}(2) & p_{32}(2) & p_{33}(2) \end{pmatrix}$$

**Theorem 1.2.1.** Let  $i, j \in S$  be states of a Markov chain with transition matrix  $\mathbf{P}$ . Then

$$p_{ij}(n) = (\mathbf{P}^n)_{ij}$$

*Proof.* We will proceed by induction on  $n$ . The theorem certainly holds for  $n = 1$  by definition of the transition matrix  $\mathbf{P}$ . Now assume that the result holds for some  $n \geq 1$ . Then

$$\begin{aligned}
p_{ij}(n+1) &= P(X_{n+1} = j | X_0 = i) \\
&= \sum_{k \in S} P(X_{n+1} = j | X_n = k) P(X_n = k | X_0 = i) \\
&= \sum_{k \in S} p_{kj} p_{ik}(n) \\
&= \sum_{k \in S} p_{kj} (\mathbf{P}^n)_{ik} \\
&= (\mathbf{P}^{n+1})_{ij}
\end{aligned}$$

□

### 1.3 State Probability Distribution

Suppose a Markov chain  $\{X_n \in S | n \in T\}$  has a finite state space  $S = \{s_1, s_2, \dots\}$ . Then each random variable  $X_n$  has a state probability distribution that can be represented using

a  $k$ -length row vector. For instance, consider the probability vector  $\vec{\pi}$  which contains the starting probability distribution of  $X_0$ .

$$\vec{\pi}^T = \begin{pmatrix} \pi_1 \\ \pi_2 \\ \vdots \\ \pi_k \end{pmatrix} = \begin{pmatrix} P(X_0 = s_1) \\ P(X_0 = s_2) \\ \vdots \\ P(X_0 =) \end{pmatrix}$$

Using the probability distribution of  $X_0$ , we can determine the probability distribution of  $X_1$ .

$$\begin{aligned} P(X_1 = j) &= \sum_{i \in S} P(X_1 = j \cap X_0 = i) \\ &= \sum_{i \in S} P(X_1 = j | X_0 = i) P(X_0 = i) \\ &= \sum_{i \in S} p_{ij} \pi_i \\ &= (\vec{\pi} P)_j \end{aligned}$$

Therefore

$$(\vec{\pi} P)^T = \begin{pmatrix} P(X_1 = s_1) \\ P(X_1 = s_2) \\ \vdots \\ P(X_1 =) \end{pmatrix}$$

Likewise, we can use a similar approach to find the probability distribution of  $X_n$  given the starting probability distribution of  $X_0$ .

$$\begin{aligned} P(X_n = j) &= \sum_{i \in S} P(X_n = j \cap X_0 = i) \\ &= \sum_{i \in S} P(X_n = j | X_0 = i) P(X_0 = i) \\ &= \sum_{i \in S} p_{ij}(n) \pi_i \\ &= \sum_{i \in S} (P^n)_{ij} \pi_i \\ &= (\vec{\pi} P^n)_j \end{aligned}$$

Therefore

$$(\vec{\pi}P^n)^T = \begin{pmatrix} P(X_n = s_1) \\ P(X_n = s_2) \\ \vdots \\ P(X_n =) \end{pmatrix}$$

## 1.4 Accessibility and Communication

**Definition 1.4.1.** A state  $j$  is *accessible* from another state  $i$  if there exists some  $n$  for which

$$p_{ij}(n) > 0$$

Moreover, if  $i$  and  $j$  are both *accessible* to each other, then they are said to *communicate*, denoted as  $i \leftrightarrow j$ .

**Proposition 1.4.1.** Communication is considered to be an equivalence relationship.

To do so, we must verify that the relation is indeed *reflexive*, *symmetric*, and *transitive*. We will prove *transitivity* and leave the rest as exercises.

*Proof.* Let  $i, j \in S$  where  $i \leftrightarrow j$  and  $j \leftrightarrow$ . Then by definition, we know that there exist some integers  $n$  and  $m$  such that  $p_{ik}(n) > 0$  and  $p_{kj}(m) > 0$ . For  $j$  to be *accessible* from  $i$ , we need to show that  $p_{ij}(l) > 0$  for some integer  $l$ . Consider the case where  $l = n + m$ .

$$\begin{aligned} p_{ij}(n+m) &= P(X_{n+m} = j | X_0 = i) \\ &= \sum_{k=1}^{|S|} P(X_{n+m} = j \cap X_n = | X_0 = i) \\ &= \sum_{k=1}^{|S|} \frac{P(X_{n+m} = j \cap X_n = \cap X_0 = i)}{P(X_0 = i)} \quad \text{Bayes' Theorem} \\ &= \sum_{k=1}^{|S|} \frac{P(X_{n+m} = j | X_n = \cap X_0 = i) P(X_n = \cap X_0 = i)}{P(X_0 = i)} \\ &= \sum_{k=1}^{|S|} P(X_{n+m} = j | X_n = \cap X_0 = i) P(X_n = | X_0 = i) \\ &= \sum_{k=1}^{|S|} P(X_{n+m} = j | X_n =) P(X_n = | X_0 = i) \quad \text{Markov Property} \\ &= \sum_{k=1}^{|S|} p_{kj}(m) p_{ik}(n) \end{aligned}$$

By assumption, there exists at least one intermediate state  $k$  that communicates both with  $i$  and  $j$  (i.e.  $p_{ik}(n) > 0$  and  $p_{kj}(m) > 0$ ), then the following inequality holds true only for the *communicating* intermediate state  $k$ .

$$p_{ij}(n+m) \geq p_{ik}(m) p_{kj}(n) > 0$$

Hence  $j$  is accessible from  $i$ . A similar argument can be made in the other direction to show that  $i$  is accessible from  $j$ , thereby proving  $i \leftrightarrow j$ .  $\square$

As a side note, we say that the *communication classes* of a Markov Process are the equivalence classes of states under communication.

## 1.5 State Classification

For any Markov chain, we classify each state according to the following definitions.

**Definition 1.5.1.** A state  $i \in S$  is called *recurrent* if

$$P(X_n = i \text{ for infinitely many } n) = 1$$

**Definition 1.5.2.** A state  $i \in S$  is called *transient* if

$$P(X_n = i \text{ for infinitely many } n) = 0$$

A *recurrent* state has the property that a Markov chain starting at that state returns to it infinitely often, with probability 1. A *transient* state however has the property that a Markov chain starting at that state returns to it finitely often, with probability 1.

**Theorem 1.5.1.** Let  $i \in S$  be a state of a Markov chain. Denote by  $f_{ii}$  the probability that a Markov chain starting at  $i$  returns to  $i$  at least once, that is

$$f_{ii} := P(X_n = i \text{ for some } n \in \mathbb{N} | X_0 = i)$$

Then,

1. The state  $i$  is *recurrent* if and only if  $f_{ii} = 1$
2. The state  $i$  is *transient* if and only if  $f_{ii} < 1$

**Theorem 1.5.2.** Let  $i, j \in S$  be states of a Markov chain.

1. If  $i$  is a *recurrent* state and  $i \leftrightarrow j$ , then  $j$  is also *recurrent*.
2. If  $i$  is a *transient* state and  $i \leftrightarrow j$ , then  $j$  is also *transient*.

*Proof.* We leave (2) as an exercise and prove (1) by contradiction. Suppose  $j$  is a *recurrent* state. Since  $i$  communicates with  $j$ , there must exist  $r, s \in \mathbb{N}$  for which  $p_{ji}(r) > 0$  and  $p_{ij}(s) > 0$ . Moreover, for all  $n \in \mathbb{N}$  it holds that

$$p_{jj}(r + n + s) \geq p_{ji}(r)p_{ii}(n)p_{ij}(s)$$

Hence,

$$\sum_{n=1}^{\infty} p_{ii}(n) \leq \frac{1}{p_{ji}(r)p_{ij}(s)} \sum_{n=1}^{\infty} p_{jj}(r + n + s) \leq \frac{1}{p_{ji}(r)p_{ij}(s)} \sum_{n=1}^{\infty} p_{jj}(n) < \infty$$

where the last inequality holds since  $j$  is transient. Therefore,  $i$  is also transient which is a contradiction.  $\square$

then  $i$  is said to be *recurrent* if  $f_{ii} = 1$ , and *transient* if  $f_{ii} < 1$ . This means that if a process starts at a *recurrent* state, then there must exist some  $n$  steps for which the process returns to that state again. When that happens, the memoryless and time-homogeneous properties ensure that the process will continue to return repeatedly to that recurrent state in the future since  $f_{ii} = 1$  every time the process reaches that state. Therefore, the recurrent state will be visited infinitely many times. On the other hand, if the process starts at a *transient* state, then it will continue to return to that state with probability

$f_{ii}$  every time it reaches it, until it is no longer able to return anymore with probability  $1 - f_{ii}$ . Subsequently, we observe that the number of times  $N$  that the transient state is visited follows a geometric distribution with "success" probability  $1 - f_{ii}$ , which is the probability that the process can no longer revisit the transient state  $i$ . If we count  $X_0 = i$  as the first visit to  $i$ , and define  $N_i$  as the number of visits to  $i$

$$P(N_i = k | X_0 = i) = f_{ii}^{k-1}(1 - f_{ii}), \quad k \geq 1$$

The expected number of visits to the transient state  $i$  given that the process starts at  $i$  can be determined

$$\begin{aligned} E[N_i | X_0 = i] &= \sum_{k=1}^{\infty} k f_{ii}^{k-1} (1 - f_{ii}) \\ &= (1 - f_{ii}) \sum_{k=1}^{\infty} k f_{ii}^{k-1} \\ &= (1 - f_{ii}) \left( \frac{d}{df_{ii}} \sum_{k=1}^{\infty} f_{ii}^k \right) \\ &= (1 - f_{ii}) \left( \frac{d}{df_{ii}} \frac{f_{ii}}{1 - f_{ii}} \right) \\ &= (1 - f_{ii}) \frac{1}{(1 - f_{ii})^2} \\ &= \frac{1}{1 - f_{ii}} \end{aligned}$$

Although this equation is valid, the value of  $f_{ii}$  is fairly difficult to calculate though possible. Alternatively, let  $I_n$  be the indicator random variable for the event  $X_n = i$ . In other words, the indicator returns 1 if the event satisfied and 0 if it is not, thereby acting as a "counter" for the number of times the process returns to  $i$ .

$$N_i = \sum_{n=0}^{\infty} I_n$$

Then the expected number of visits to the transient state  $i$  given that the process starts at  $i$  can be expressed as such

$$\begin{aligned} E[N_i | X_0 = i] &= E \left[ \sum_{n=0}^{\infty} I_n | X_0 = i \right] \\ &= \sum_{n=0}^{\infty} E[I_n | X_0 = i] && \text{By linearity of expectation} \\ &= \sum_{n=0}^{\infty} P(X_n = i | X_0 = i) \\ &= \sum_{n=0}^{\infty} p_{ii}(n) \\ &= \sum_{n=0}^{\infty} (P^n)_{ii} \end{aligned}$$



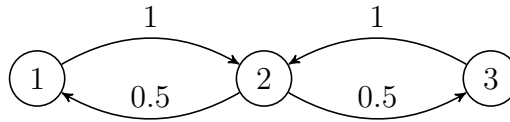
Therefore, we can use the transition matrix  $\mathbf{P}$  to determine the mean number of visits to a transient state.

## 1.6 Convergence to Equilibrium

By combining individual states in a process, we obtain different types of Markov chains; some of them have stabilizing long term behaviors while others do not. Note that by "stabilizing long term behavior", we mean that the process gradually converges towards a unique steady state distribution, regardless of the initial conditions. This equilibrium distribution will then help us predict the long term proportion of time spent in each state. We will first look at examples of processes that do not have a stable long term behavior.

### 1.6.1 Periodic Markov Chains

A state in a Markov chain is said to be periodic if the process can only return to that state at multiples of an integer greater than 1. It should also be noted that periodicity is a *class property*, meaning that if one state is periodic, then every other state in its communication class is also periodic. To illustrate, consider the following periodic Markov chain.



If the process starts at state  $s_1$ , then we see that it can only return to that state in an even number of steps. The same can be said about  $s_3$ , whereas  $s_2$  strictly has a period of 2 steps. Moreover, consider the transition matrix of this process.

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0.5 & 0 & 0.5 \\ 0 & 1 & 0 \end{pmatrix}$$

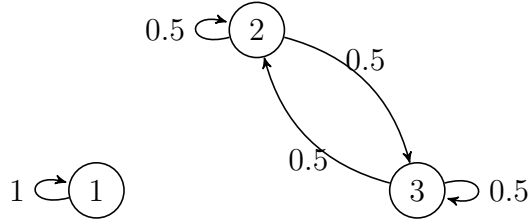
When we take successive powers of the transition matrix, it can be observed that the resulting matrix alternates between  $\mathbf{P}^{n_{odd}}$  and  $\mathbf{P}^{n_{even}}$ .

$$\mathbf{P}^{n_{odd}} = \begin{pmatrix} 0 & 1 & 0 \\ 0.5 & 0 & 0.5 \\ 0 & 1 & 0 \end{pmatrix} ; \mathbf{P}^{n_{even}} = \begin{pmatrix} 0.5 & 0 & 0.5 \\ 0 & 1 & 0 \\ 0.5 & 0 & 0.5 \end{pmatrix}$$

The  $n$ -step transition matrix  $\mathbf{P}^n$  does not converge to some equilibrium matrix  $\sigma$  as  $n \rightarrow \infty$ . Therefore, the long term state distribution of a periodic process cannot be constant

### 1.6.2 Reducible Markov chains

A Markov chain is said to be *reducible* if it has more than one communication class. This implies that not every state in the state space is able to communicate with each other. To illustrate, consider the following reducible Markov chain.



In this example, there are two communication classes, namely  $\{s_1\}$  and  $\{s_2, s_3\}$ . As a result, the long term behavior of the process depends entirely on the initial state of the process. For instance, if the process starts at  $s_1$ , then it will stay there forever, but if it starts either at  $s_2$  or  $s_3$ , then the process will stay in that communication class forever. Therefore, the stationary probability distribution of a reducible Markov chain depends on its starting distribution  $\vec{\pi}$  (More on this in the next section).

### 1.6.3 Regular Markov chains

We now look at Markov chains that do possess an equilibrium distribution, also known as *regular* Markov chains. Contrary to the previous two types of Markov chains we have seen, a regular Markov chain must be *aperiodic*, *irreducible*, and also *positive recurrent*. In other words, this means that the process must only have states that are visited aperiodically, one communication class for the entire state space, and a mean number of visits to every state that is infinite.

One easy way to check if a Markov chain obeys these conditions is by finding some power of the  $n$ -step transition matrix  $\mathbf{P}^n$  for which the matrix contains only strictly positive entries. As such, for that number  $n$ , every  $n$ -step transition probability  $p_{ij}(n)$  has a strictly positive value, thereby demonstrating that the process is *irreducible* since every state communicates with each other and belongs to a single communication class. Moreover, this method also works to show that the Markov chain is aperiodic since every  $n$ -step self-transition probability is greater than 0 (i.e.  $p_{ii}(n) > 0$ ). This means that the process must again be able to perform this self-transition in the next step  $p_{ii}(n+1) > 0$ , thereby breaking the periodicity of the process. Finally, knowing that the process is irreducible, this implies that every state in the process must be recurrent such that the mean number of visits to every state is infinite. Hence, positive recurrence is a property that is always present in a finite irreducible Markov chain. In brief, regular Markov chains are the only processes for which the steady-state distribution both exists and is nontrivial. We will examine how these equilibrium distributions can be determined in the next section.

## 1.7 Steady-State Distribution

Recall from a previous section that the state probability distribution of  $X_n$  given the starting distribution  $X_0$  can be expressed as such

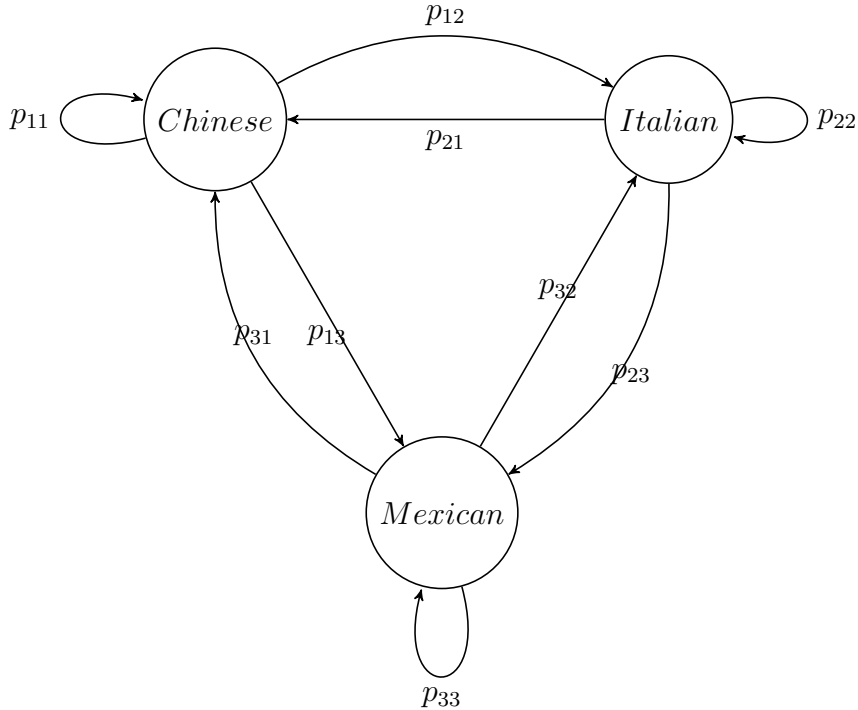
$$(\vec{\pi}P^n)^T = \begin{pmatrix} P(X_n = s_1) \\ P(X_n = s_2) \\ \vdots \\ P(X_n = s_k) \end{pmatrix}$$

As mentioned, for regular Markov chains, we can expect to find a stationary distribution as  $n \rightarrow \infty$ . However, instead of computing large powers of the transition matrix, we can solve the following matrix equation to find the equilibrium distribution  $\vec{\pi}^*$

$$\begin{aligned} \vec{\pi}^* &= \vec{\pi}^* P \\ \vec{\pi}^* (I_k - P) &= \vec{0} \end{aligned}$$

where  $I_k$  is a  $k$ -sized identity matrix. As a result, the steady-state distribution vector is simply a left eigenvector of the transition matrix with corresponding eigenvalue 1.

\*Example 1: Restaurants Every day, a hungry customer eats at one of three restaurants, each serving a different cuisine: Chinese, Italian, and Mexican, conveniently denoted as states 1, 2, and 3 respectively. The customer's restaurant choice for the next day is probabilistically determined by the restaurant he visits on the current day (see Figure below).



For this Markov chain to be regular, we will consider the following transition matrix, which is also the default matrix implemented in the Streamlit simulation.

$$\mathbf{P} = \begin{pmatrix} 0.5 & 0.2 & 0.3 \\ 0.6 & 0.3 & 0.1 \\ 0.4 & 0.5 & 0.1 \end{pmatrix}$$

Since the one-step transition matrix already has only strictly positive entries, this process is considered to be regular and therefore it must have an equilibrium distribution.

In the Python code, the theoretical equilibrium distribution is found by computing the left eigenvector of the transition matrix with corresponding eigenvalue 1, which is then compared to the experimental distribution that is found by computing successive powers of the transition matrix. As the process moves forward in steps, it can be observed that the theoretical and experimental distributions start to match as the initial condition of the process quickly becomes insignificant.

## 2 Absorbing Markov chain

We now begin our study of *absorbing* Markov chains, which are almost polar opposites of *regular* Markov chains. To contextualize, if a process is in state  $i$  and is unable to leave it, then that state is considered to be an *absorbing* state. Additionally, if it is possible to go from any *non-absorbing* state to an absorbing state in one or more steps, then the entire process is considered to be an *absorbing* Markov chain. Notice that *absorbing* states are also *recurrent*, whereas non-absorbing states are *transient* since the process can be absorbed starting from any non-absorbing state.

### Canonical Form

The canonical form is a representation of the transition matrix  $\mathbf{P}$  into 4 block matrices. Suppose the transition matrix of an absorbing Markov chain has  $t$  transient states and  $r$  absorbing states. Then the canonical form of the transition matrix  $\mathbf{P}$  is

$$P = \left( \begin{array}{c|c} Q & R \\ \hline 0 & I_r \end{array} \right)$$

where  $Q$  is a  $t \times t$  matrix,  $0$  is an  $r \times t$  zero matrix,  $R$  is a  $t \times r$  nonzero matrix, and  $I_r$  is a  $r \times r$  matrix. Since the matrix  $Q$  only contains transient states, it summarizes the transition probabilities between non absorbing states. The matrix  $R$  contains transient and recurrent states, thereby representing the transition probabilities from non-absorbing states to absorbing ones. Next, we know that it is impossible to go from an absorbing state to a non-absorbing state, hence the  $0$  matrix. And finally, the identity matrix  $I_r$  contains the self-transition probabilities for the absorbing states which are 1.

Moreover, a simple exercise shows that the  $n$ th power of the canonical form matrix yields

$$P^n = \left( \begin{array}{c|c} Q^n & R + QR + Q^2R + \dots + Q^{n-1}R \\ \hline 0 & I_r \end{array} \right)$$

$$P^n = \left( \begin{array}{c|c} Q^n & \sum_{k=1}^n Q^{k-1} R \\ \hline 0 & I_r \end{array} \right)$$

Notice that we obtain the  $n$ -step transition probabilities between transient states under  $Q^n$ . Even more interestingly, we observe that the top-right matrix expression is closely related to a geometric distribution. Now, consider the  $n$ -step transition matrix as  $n$  approaches infinity

$$\lim_{n \rightarrow \infty} P^n = \left( \begin{array}{c|c} \lim_{n \rightarrow \infty} Q^n & \sum_{k=1}^{\infty} Q^{k-1} R \\ \hline 0 & I_r \end{array} \right)$$

First, let us examine the top-left expression (i.e.  $\lim_{n \rightarrow \infty} Q^n$ ). Since it is possible to go from any non-absorbing state to an absorbing one, this means that the sum of every row in  $Q$  must be smaller than 1. As a result, the largest eigenvalue of  $Q$  must also be smaller than 1, and therefore  $Q^n \rightarrow 0$  as  $n \rightarrow \infty$ . In other words, the probability that an absorbing Markov chain will be absorbed is 1.

As for the top-right expression (i.e.  $\lim_{n \rightarrow \infty} \sum_{k=1}^{\infty} Q^{k-1} R$ ), it contains the absorbing probabilities of the Markov chain, which will be further discussed in the next section.

## The Fundamental Matrix

For any absorbing Markov chain, the *fundamental matrix* denoted  $N$  provides the expected number of visits to a non-absorbing state.

$$N = \sum_{n=0}^{\infty} Q^n = (I - Q)^{-1}$$

More specifically, the  $(i,j)$  entry of the fundamental matrix  $N$  gives the expected number of visits to the transient state  $j$  given that the process starts at the transient state  $i$ . This can be shown by starting from the definition of expectation and by defining the indicator random variable  $I_n$  for the event  $\{X_n = j\}$ . Recall that a very similar derivation was already shown on page 7.

$$\begin{aligned} E[N_j | X_0 = i] &= E \left[ \sum_{n=0}^{\infty} I_n | X_0 = i \right] \\ &= \sum_{n=0}^{\infty} E[I_n | X_0 = i] \\ &= \sum_{n=0}^{\infty} P(X_n = j | X_0 = i) \\ &= \sum_{n=0}^{\infty} q_{ij}(n) \\ &= \sum_{n=0}^{\infty} (Q^n)_{ij} \\ &= N_{ij} \end{aligned}$$

From these above equations, we can further simplify our limiting transition matrix

$$\lim_{n \rightarrow \infty} P^n = \left( \begin{array}{c|c} 0 & NR \\ \hline 0 & I_r \end{array} \right)$$

If we let  $B = NR$ , then the  $(i,j)$  entry of matrix  $B$  gives the probability that the process will be absorbed at the absorbing state  $j$  given that it started at the transient state  $i$ . To show that this is true, by the law of total probability, we must consider every possible route from  $i$  to  $j$  through intermediate transient states  $k$ , and also for all possible number of steps.

$$\begin{aligned} B_{ij} &= \sum_n \sum_k q_{ik}(n) r_{kj} \\ &= \sum_n \sum_k (Q^n)_{ik} r_{kj} \\ &= \sum_k n_{ik} r_{kj} \\ &= (NR)_{ij} \end{aligned}$$

Finally, we can even use the fundamental matrix  $N$  to determine the expected time to absorption given that the process starts at a transient state  $i$ . To show this, let  $t$  be a column vector such that its entries  $t_i$  represent the expected time to absorption given that the process starts at  $i$ . Then

$$t = N1$$

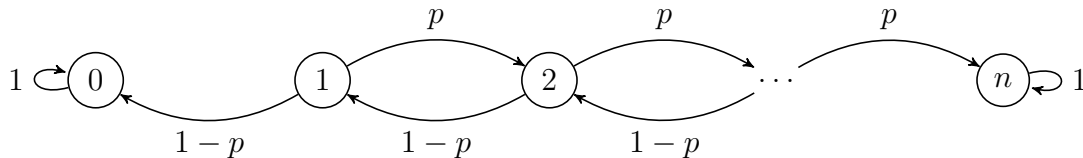
where  $1$  is a column vector of 1s. To visualize the calculation,

$$t_i = \sum_k N_{ik}$$

Therefore, we are adding the expected visits to all non-absorbing states given that the process starts at  $i$ , which is also indicative of the total expected number of steps until the process is absorbed.

### Example 2: Gambler's Ruin

A gambler has an initial wealth of  $k$  dollars and bets 1\$ every round with probability  $p$  of winning each round. The gambler keeps playing until his wealth is either emptied or reaches a value  $n$  (see Figure 2).



The states  $s_0$  and  $s_n$  are considered *absorbing* whereas the states  $s_1, s_2, \dots, s_{n-1}$  are *transient*. Furthermore, the transition probabilities can be summarized using a transition matrix  $\mathbf{P}$

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1-p & 0 & p & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1-p & 0 & p & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-p & 0 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & p & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 1-p & 0 & p & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1-p & 0 & p \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 \end{pmatrix} \quad (2)$$

For the sake of simplicity, we will consider the following transition matrix that contains 3 transient states and 2 absorbing states.

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (3)$$

The canonical form of the transition matrix

$$A = \left( \begin{array}{ccc|cc} 0 & 1/2 & 0 & 1/2 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array} \right) \quad (4)$$

Therefore

$$\mathbf{Q} = \begin{pmatrix} 0 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 \end{pmatrix}; \mathbf{R} = \begin{pmatrix} 1/2 & 0 \\ 0 & 0 \\ 0 & 1/2 \end{pmatrix} \quad (5)$$

The fundamental matrix is given as

$$N = (I - Q)^{-1} = \begin{pmatrix} 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 3/2 \end{pmatrix} \quad (6)$$

We now find the  $t$  column vector whose entries  $t_i$  contain the expected time to absorption given that the process starts at  $i$

$$\mathbf{t} = \begin{pmatrix} 3 \\ 4 \\ 3 \end{pmatrix} \quad (7)$$

Now that we have the theoretical results, we can use the Streamlit simulation to produce experimental results for comparison. As initial conditions, we set the target to 4 and the initial wealth to 2. Therefore, the expected number of steps until the process is absorbed is 4 (according to the second entry of the  $t$  column vector).

For a sample size of 101, it was experimentally found that the sample mean was 3.9802 and the standard deviation was 2.4248. As an exercise, we will construct a 95% confidence interval for the average number of steps to absorption. Since the population variance is unknown, we use the t-distribution to find the critical t value:  $t_{0.025,100} = 1.984$ . Then, we construct the confidence interval

$$\begin{aligned} \bar{x} - t_{0.025,100} \frac{s}{\sqrt{n}} &\leq \mu \leq \bar{x} + t_{0.025,100} \frac{s}{\sqrt{n}} \\ 3.9802 - 1.984 \frac{2.4248}{\sqrt{101}} &\leq \mu \leq 3.9802 + 1.984 \frac{2.4248}{\sqrt{101}} \\ 3.5015 &\leq \mu \leq 4.4589 \end{aligned}$$

With repeated sampling, we are 95% confident that the true mean number of games that the gambler must play until they lose or win lies between 3.5015 and 4.4589. Since  $4 \in \text{C.I.}$ , we have sufficient evidence to believe that the experimental results match the theoretical ones.

### 3 Hidden Markov Model