Chapter 11

Markov Chains

11.1 Introduction

Most of our study of probability has dealt with independent trials processes. These processes are the basis of classical probability theory and much of statistics. We have discussed two of the principal theorems for these processes: the Law of Large Numbers and the Central Limit Theorem.

We have seen that when a sequence of chance experiments forms an independent trials process, the possible outcomes for each experiment are the same and occur with the same probability. Further, knowledge of the outcomes of the previous experiments does not influence our predictions for the outcomes of the next experiment. The distribution for the outcomes of a single experiment is sufficient to construct a tree and a tree measure for a sequence of n experiments, and we can answer any probability question about these experiments by using this tree measure.

Modern probability theory studies chance processes for which the knowledge of previous outcomes influences predictions for future experiments. In principle, when we observe a sequence of chance experiments, all of the past outcomes could influence our predictions for the next experiment. For example, this should be the case in predicting a student's grades on a sequence of exams in a course. But to allow this much generality would make it very difficult to prove general results.

In 1907, A. A. Markov began the study of an important new type of chance process. In this process, the outcome of a given experiment can affect the outcome of the next experiment. This type of process is called a Markov chain.

Specifying a Markov Chain

We describe a Markov chain as follows: We have a set of *states*, $S = \{s_1, s_2, \ldots, s_r\}$. The process starts in one of these states and moves successively from one state to another. Each move is called a *step*. If the chain is currently in state s_i , then it moves to state s_j at the next step with a probability denoted by p_{ij} , and this probability does not depend upon which states the chain was in before the current state.

The probabilities p_{ij} are called *transition probabilities*. The process can remain in the state it is in, and this occurs with probability p_{ii} . An initial probability distribution, defined on S, specifies the starting state. Usually this is done by specifying a particular state as the starting state.

R. A. Howard¹ provides us with a picturesque description of a Markov chain as a frog jumping on a set of lily pads. The frog starts on one of the pads and then jumps from lily pad to lily pad with the appropriate transition probabilities.

Example 11.1 According to Kemeny, Snell, and Thompson,² the Land of Oz is blessed by many things, but not by good weather. They never have two nice days in a row. If they have a nice day, they are just as likely to have snow as rain the next day. If they have snow or rain, they have an even chance of having the same the next day. If there is change from snow or rain, only half of the time is this a change to a nice day. With this information we form a Markov chain as follows. We take as states the kinds of weather R, N, and S. From the above information we determine the transition probabilities. These are most conveniently represented in a square array as

$$\mathbf{P} = \begin{array}{ccc} \mathbf{R} & \mathbf{N} & \mathbf{S} \\ \mathbf{P} = \begin{array}{ccc} \mathbf{R} \\ \mathbf{N} \\ \mathbf{S} \end{array} \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{array} \right)$$

Transition Matrix

The entries in the first row of the matrix \mathbf{P} in Example 11.1 represent the probabilities for the various kinds of weather following a rainy day. Similarly, the entries in the second and third rows represent the probabilities for the various kinds of weather following nice and snowy days, respectively. Such a square array is called the *matrix of transition probabilities*, or the *transition matrix*.

We consider the question of determining the probability that, given the chain is in state *i* today, it will be in state *j* two days from now. We denote this probability by $p_{ij}^{(2)}$. In Example 11.1, we see that if it is rainy today then the event that it is snowy two days from now is the disjoint union of the following three events: 1) it is rainy tomorrow and snowy two days from now, 2) it is nice tomorrow and snowy two days from now, and 3) it is snowy tomorrow and snowy two days from now. The probability of the first of these events is the product of the conditional probability that it is rainy tomorrow, given that it is rainy tomorrow. Using the transition matrix **P**, we can write this product as $p_{11}p_{13}$. The other two

¹R. A. Howard, *Dynamic Probabilistic Systems*, vol. 1 (New York: John Wiley and Sons, 1971).

²J. G. Kemeny, J. L. Snell, G. L. Thompson, *Introduction to Finite Mathematics*, 3rd ed. (Englewood Cliffs, NJ: Prentice-Hall, 1974).

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events also have probabilities that can be written as products of entries of **P**. Thus, we have

$$p_{13}^{(2)} = p_{11}p_{13} + p_{12}p_{23} + p_{13}p_{33} \; .$$

This equation should remind the reader of a dot product of two vectors; we are dotting the first row of \mathbf{P} with the third column of \mathbf{P} . This is just what is done in obtaining the 1,3-entry of the product of \mathbf{P} with itself. In general, if a Markov chain has r states, then

$$p_{ij}^{(2)} = \sum_{k=1}^{r} p_{ik} p_{kj}$$

The following general theorem is easy to prove by using the above observation and induction.

Theorem 11.1 Let **P** be the transition matrix of a Markov chain. The *ij*th entry $p_{ij}^{(n)}$ of the matrix **P**ⁿ gives the probability that the Markov chain, starting in state s_i , will be in state s_j after n steps.

Proof. The proof of this theorem is left as an exercise (Exercise 17).

Example 11.2 (Example 11.1 continued) Consider again the weather in the Land of Oz. We know that the powers of the transition matrix give us interesting information about the process as it evolves. We shall be particularly interested in the state of the chain after a large number of steps. The program **MatrixPowers** computes the powers of **P**.

We have run the program **MatrixPowers** for the Land of Oz example to compute the successive powers of **P** from 1 to 6. The results are shown in Table 11.1. We note that after six days our weather predictions are, to three-decimal-place accuracy, independent of today's weather. The probabilities for the three types of weather, R, N, and S, are .4, .2, and .4 no matter where the chain started. This is an example of a type of Markov chain called a *regular* Markov chain. For this type of chain, it is true that long-range predictions are independent of the starting state. Not all chains are regular, but this is an important class of chains that we shall study in detail later. \Box

We now consider the long-term behavior of a Markov chain when it starts in a state chosen by a probability distribution on the set of states, which we will call a *probability vector*. A probability vector with r components is a row vector whose entries are non-negative and sum to 1. If **u** is a probability vector which represents the initial state of a Markov chain, then we think of the *i*th component of **u** as representing the probability that the chain starts in state s_i .

With this interpretation of random starting states, it is easy to prove the following theorem.

$\mathbf{P}^1 =$	Rain Nice Snow	Rain .500 .500 .250	Nice .250 .000 .250	(350) (350) (350) (350) (350)
$\mathbf{P}^2 =$	Rain Nice Snow	Rain .438 .375 .375	Nice .188 .250 .188	$ \begin{array}{c} \text{Snow} \\ .375 \\ .375 \\ .438 \end{array} \right) $
$\mathbf{P}^3 =$	Rain Nice Snow	Rain .406 .406 .391	Nice .203 .188 .203	$ \begin{array}{c} \text{Snow} \\ .391 \\ .406 \\ .406 \end{array} \right) $
	Bain /	Rain	Nice	Snow 308
$\mathbf{P}^4 =$	Nice Snow (.398 .398	.199 .203 .199	(.398) (.398) (.402)
$\mathbf{P}^4 =$ $\mathbf{P}^5 =$	Rain Nice Snow	.402 .398 .398 Rain .400 .400 .399	.199 .203 .199 Nice .200 .199 .200	$ \begin{array}{c} .398 \\ .398 \\ .402 \end{array} \right) $ Snow $ \begin{array}{c} .399 \\ .400 \\ .400 \end{array} \right) $

Table 11.1: Powers of the Land of Oz transition matrix.

Theorem 11.2 Let **P** be the transition matrix of a Markov chain, and let **u** be the probability vector which represents the starting distribution. Then the probability that the chain is in state s_i after n steps is the *i*th entry in the vector

$$\mathbf{u}^{(n)} = \mathbf{u}\mathbf{P}^n$$

Proof. The proof of this theorem is left as an exercise (Exercise 18).

We note that if we want to examine the behavior of the chain under the assumption that it starts in a certain state s_i , we simply choose **u** to be the probability vector with *i*th entry equal to 1 and all other entries equal to 0.

Example 11.3 In the Land of Oz example (Example 11.1) let the initial probability vector **u** equal (1/3, 1/3, 1/3). Then we can calculate the distribution of the states after three days using Theorem 11.2 and our previous calculation of \mathbf{P}^3 . We obtain

$$\mathbf{u}^{(3)} = \mathbf{u}\mathbf{P}^{3} = (1/3, 1/3, 1/3) \begin{pmatrix} .406 & .203 & .391 \\ .406 & .188 & .406 \\ .391 & .203 & .406 \end{pmatrix}$$
$$= (.401, .188, .401) .$$

Examples

The following examples of Markov chains will be used throughout the chapter for exercises.

Example 11.4 The President of the United States tells person A his or her intention to run or not to run in the next election. Then A relays the news to B, who in turn relays the message to C, and so forth, always to some new person. We assume that there is a probability a that a person will change the answer from yes to no when transmitting it to the next person and a probability b that he or she will change it from no to yes. We choose as states the message, either yes or no. The transition matrix is then

$$\mathbf{P} = \frac{\text{yes}}{\text{no}} \begin{pmatrix} 1-a & a \\ b & 1-b \end{pmatrix} \,.$$

The initial state represents the President's choice.

Example 11.5 Each time a certain horse runs in a three-horse race, he has probability 1/2 of winning, 1/4 of coming in second, and 1/4 of coming in third, independent of the outcome of any previous race. We have an independent trials process,

but it can also be considered from the point of view of Markov chain theory. The transition matrix is

$$\mathbf{P} = \mathbf{P} \begin{pmatrix} .5 & .25 & .25 \\ .5 & .25 & .25 \\ .5 & .25 & .25 \end{pmatrix}.$$

Example 11.6 In the Dark Ages, Harvard, Dartmouth, and Yale admitted only male students. Assume that, at that time, 80 percent of the sons of Harvard men went to Harvard and the rest went to Yale, 40 percent of the sons of Yale men went to Yale, and the rest split evenly between Harvard and Dartmouth; and of the sons of Dartmouth men, 70 percent went to Dartmouth, 20 percent to Harvard, and 10 percent to Yale. We form a Markov chain with transition matrix

$$\mathbf{P} = \begin{array}{ccc} H & Y & D \\ H & (.8 & .2 & 0) \\ Y & (.3 & .4 & .3) \\ D & (.2 & .1 & .7) \end{array} .$$

Example 11.7 Modify Example 11.6 by assuming that the son of a Harvard man always went to Harvard. The transition matrix is now

$$\mathbf{P} = \begin{array}{ccc} H & Y & D \\ H & \begin{pmatrix} 1 & 0 & 0 \\ .3 & .4 & .3 \\ D & 2 & .1 & .7 \end{array} \right) \, .$$

Example 11.8 (Ehrenfest Model) The following is a special case of a model, called the Ehrenfest model,³ that has been used to explain diffusion of gases. The general model will be discussed in detail in Section 11.5. We have two urns that, between them, contain four balls. At each step, one of the four balls is chosen at random and moved from the urn that it is in into the other urn. We choose, as states, the number of balls in the first urn. The transition matrix is then

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 0 & 1 & 0 & 0 & 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1/4 & 0 & 3/4 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 3/4 & 0 & 1/4 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

³P. and T. Ehrenfest, "Über zwei bekannte Einwände gegen das Boltzmannsche H-Theorem," *Physikalishce Zeitschrift*, vol. 8 (1907), pp. 311-314.

Example 11.9 (Gene Model) The simplest type of inheritance of traits in animals occurs when a trait is governed by a pair of genes, each of which may be of two types, say G and g. An individual may have a GG combination or Gg (which is genetically the same as gG) or gg. Very often the GG and Gg types are indistinguishable in appearance, and then we say that the G gene dominates the g gene. An individual is called *dominant* if he or she has GG genes, *recessive* if he or she has gg, and *hybrid* with a Gg mixture.

In the mating of two animals, the offspring inherits one gene of the pair from each parent, and the basic assumption of genetics is that these genes are selected at random, independently of each other. This assumption determines the probability of occurrence of each type of offspring. The offspring of two purely dominant parents must be dominant, of two recessive parents must be recessive, and of one dominant and one recessive parent must be hybrid.

In the mating of a dominant and a hybrid animal, each offspring must get a G gene from the former and has an equal chance of getting G or g from the latter. Hence there is an equal probability for getting a dominant or a hybrid offspring. Again, in the mating of a recessive and a hybrid, there is an even chance for getting either a recessive or a hybrid. In the mating of two hybrids, the offspring has an equal chance of getting G or g from each parent. Hence the probabilities are 1/4 for GG, 1/2 for Gg, and 1/4 for gg.

Consider a process of continued matings. We start with an individual of known genetic character and mate it with a hybrid. We assume that there is at least one offspring. An offspring is chosen at random and is mated with a hybrid and this process repeated through a number of generations. The genetic type of the chosen offspring in successive generations can be represented by a Markov chain. The states are dominant, hybrid, and recessive, and indicated by GG, Gg, and gg respectively.

The transition probabilities are

$$\mathbf{P} = \begin{array}{ccc} GG & Gg & gg \\ GG & \begin{pmatrix} .5 & .5 & 0 \\ .25 & .5 & .25 \\ gg & \begin{pmatrix} 0 & .5 & .5 \end{pmatrix} \end{array}.$$

Example 11.10 Modify Example 11.9 as follows: Instead of mating the oldest offspring with a hybrid, we mate it with a dominant individual. The transition matrix is

$$\mathbf{P} = \begin{array}{ccc} GG & Gg & gg \\ GG \\ Gg \\ gg \end{array} \begin{pmatrix} 1 & 0 & 0 \\ .5 & .5 & 0 \\ 0 & 1 & 0 \end{array} \end{pmatrix}.$$

Example 11.11 We start with two animals of opposite sex, mate them, select two of their offspring of opposite sex, and mate those, and so forth. To simplify the example, we will assume that the trait under consideration is independent of sex.

Here a state is determined by a pair of animals. Hence, the states of our process will be: $s_1 = (GG, GG), s_2 = (GG, Gg), s_3 = (GG, gg), s_4 = (Gg, Gg), s_5 = (Gg, gg), and s_6 = (gg, gg).$

We illustrate the calculation of transition probabilities in terms of the state s_2 . When the process is in this state, one parent has GG genes, the other Gg. Hence, the probability of a dominant offspring is 1/2. Then the probability of transition to s_1 (selection of two dominants) is 1/4, transition to s_2 is 1/2, and to s_4 is 1/4. The other states are treated the same way. The transition matrix of this chain is:

		GG, GG	GG, Gg	GG,gg	Gg, Gg	Gg,gg	gg,gg	
	GG, GG	1.000	.000	.000	.000	.000	.000 \	
	GG,Gg	.250	.500	.000	.250	.000	.000	
\mathbf{P}^1 –	GG,gg	.000	.000	.000	1.000	.000	.000	
1 –	Gg,Gg	.062	.250	.125	.250	.250	.062	
	Gg,gg	.000	.000	.000	.250	.500	.250	
	gg,gg	.000	.000	.000	.000	.000	1.000	

Example 11.12 (Stepping Stone Model) Our final example is another example that has been used in the study of genetics. It is called the *stepping stone* model.⁴ In this model we have an *n*-by-*n* array of squares, and each square is initially any one of *k* different colors. For each step, a square is chosen at random. This square then chooses one of its eight neighbors at random and assumes the color of that neighbor. To avoid boundary problems, we assume that if a square *S* is on the left-hand boundary, say, but not at a corner, it is adjacent to the square *T* on the right-hand boundary in the same row as *S*, and *S* is also adjacent to the squares just above and below *T*. A similar assumption is made about squares on the upper and lower boundaries. (These adjacencies are much easier to understand if one imagines making the array into a cylinder by gluing the top and bottom edge together, and then making the cylinder into a doughnut by gluing the two circular boundaries together.) With these adjacencies, each square in the array is adjacent to exactly eight other squares.

A state in this Markov chain is a description of the color of each square. For this Markov chain the number of states is k^{n^2} , which for even a small array of squares is enormous. This is an example of a Markov chain that is easy to simulate but difficult to analyze in terms of its transition matrix. The program **SteppingStone** simulates this chain. We have started with a random initial configuration of two colors with n = 20 and show the result after the process has run for some time in Figure 11.2.

⁴S. Sawyer, "Results for The Stepping Stone Model for Migration in Population Genetics," Annals of Probability, vol. 4 (1979), pp. 699–728.



Figure 11.1: Initial state of the stepping stone model.



Figure 11.2: State of the stepping stone model after 10,000 steps.

This is an example of an *absorbing* Markov chain. This type of chain will be studied in Section 11.2. One of the theorems proved in that section, applied to the present example, implies that with probability 1, the stones will eventually all be the same color. By watching the program run, you can see that territories are established and a battle develops to see which color survives. At any time the probability that a particular color will win out is equal to the proportion of the array of this color. You are asked to prove this in Exercise 11.2.32.

Exercises

- 1 It is raining in the Land of Oz. Determine a tree and a tree measure for the next three days' weather. Find $\mathbf{w}^{(1)}, \mathbf{w}^{(2)}$, and $\mathbf{w}^{(3)}$ and compare with the results obtained from \mathbf{P}, \mathbf{P}^2 , and \mathbf{P}^3 .
- **2** In Example 11.4, let a = 0 and b = 1/2. Find **P**, **P**², and **P**³. What would **P**ⁿ be? What happens to **P**ⁿ as *n* tends to infinity? Interpret this result.
- **3** In Example 11.5, find **P**, \mathbf{P}^2 , and \mathbf{P}^3 . What is \mathbf{P}^n ?

- **4** For Example 11.6, find the probability that the grandson of a man from Harvard went to Harvard.
- 5 In Example 11.7, find the probability that the grandson of a man from Harvard went to Harvard.
- 6 In Example 11.9, assume that we start with a hybrid bred to a hybrid. Find $\mathbf{w}^{(1)}$, $\mathbf{w}^{(2)}$, and $\mathbf{w}^{(3)}$. What would $\mathbf{w}^{(n)}$ be?
- 7 Find the matrices \mathbf{P}^2 , \mathbf{P}^3 , \mathbf{P}^4 , and \mathbf{P}^n for the Markov chain determined by the transition matrix $\mathbf{P} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Do the same for the transition matrix $\mathbf{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Interpret what happens in each of these processes.
- 8 A certain calculating machine uses only the digits 0 and 1. It is supposed to transmit one of these digits through several stages. However, at every stage, there is a probability p that the digit that enters this stage will be changed when it leaves and a probability q = 1 p that it won't. Form a Markov chain to represent the process of transmission by taking as states the digits 0 and 1. What is the matrix of transition probabilities?
- **9** For the Markov chain in Exercise 8, draw a tree and assign a tree measure assuming that the process begins in state 0 and moves through two stages of transmission. What is the probability that the machine, after two stages, produces the digit 0 (i.e., the correct digit)? What is the probability that the machine never changed the digit from 0? Now let p = .1. Using the program **MatrixPowers**, compute the 100th power of the transition matrix. Interpret the entries of this matrix. Repeat this with p = .2. Why do the 100th powers appear to be the same?
- 10 Modify the program MatrixPowers so that it prints out the average \mathbf{A}_n of the powers \mathbf{P}^n , for n = 1 to N. Try your program on the Land of Oz example and compare \mathbf{A}_n and \mathbf{P}^n .
- 11 Assume that a man's profession can be classified as professional, skilled laborer, or unskilled laborer. Assume that, of the sons of professional men, 80 percent are professional, 10 percent are skilled laborers, and 10 percent are unskilled laborers. In the case of sons of skilled laborers, 60 percent are skilled laborers, 20 percent are professional, and 20 percent are unskilled. Finally, in the case of unskilled laborers, 50 percent of the sons are unskilled laborers, and 25 percent each are in the other two categories. Assume that every man has at least one son, and form a Markov chain by following the profession of a randomly chosen son of a given family through several generations. Set up the matrix of transition probabilities. Find the probability that a randomly chosen grandson of an unskilled laborer is a professional man.
- 12 In Exercise 11, we assumed that every man has a son. Assume instead that the probability that a man has at least one son is .8. Form a Markov chain

with four states. If a man has a son, the probability that this son is in a particular profession is the same as in Exercise 11. If there is no son, the process moves to state four which represents families whose male line has died out. Find the matrix of transition probabilities and find the probability that a randomly chosen grandson of an unskilled laborer is a professional man.

- 13 Write a program to compute $\mathbf{u}^{(n)}$ given \mathbf{u} and \mathbf{P} . Use this program to compute $\mathbf{u}^{(10)}$ for the Land of Oz example, with $\mathbf{u} = (0, 1, 0)$, and with $\mathbf{u} = (1/3, 1/3, 1/3)$.
- 14 Using the program MatrixPowers, find \mathbf{P}^1 through \mathbf{P}^6 for Examples 11.9 and 11.10. See if you can predict the long-range probability of finding the process in each of the states for these examples.
- 15 Write a program to simulate the outcomes of a Markov chain after n steps, given the initial starting state and the transition matrix **P** as data (see Example 11.12). Keep this program for use in later problems.
- 16 Modify the program of Exercise 15 so that it keeps track of the proportion of times in each state in n steps. Run the modified program for different starting states for Example 11.1 and Example 11.8. Does the initial state affect the proportion of time spent in each of the states if n is large?
- 17 Prove Theorem 11.1.
- 18 Prove Theorem 11.2.
- 19 Consider the following process. We have two coins, one of which is fair, and the other of which has heads on both sides. We give these two coins to our friend, who chooses one of them at random (each with probability 1/2). During the rest of the process, she uses only the coin that she chose. She now proceeds to toss the coin many times, reporting the results. We consider this process to consist solely of what she reports to us.
 - (a) Given that she reports a head on the *n*th toss, what is the probability that a head is thrown on the (n + 1)st toss?
 - (b) Consider this process as having two states, heads and tails. By computing the other three transition probabilities analogous to the one in part (a), write down a "transition matrix" for this process.
 - (c) Now assume that the process is in state "heads" on both the (n-1)st and the *n*th toss. Find the probability that a head comes up on the (n+1)st toss.
 - (d) Is this process a Markov chain?

11.2 Absorbing Markov Chains

The subject of Markov chains is best studied by considering special types of Markov chains. The first type that we shall study is called an *absorbing Markov chain*.



Figure 11.3: Drunkard's walk.

Definition 11.1 A state s_i of a Markov chain is called *absorbing* if it is impossible to leave it (i.e., $p_{ii} = 1$). A Markov chain is *absorbing* if it has at least one absorbing state, and if from every state it is possible to go to an absorbing state (not necessarily in one step).

Definition 11.2 In an absorbing Markov chain, a state which is not absorbing is called *transient*. $\hfill \Box$

Drunkard's Walk

Example 11.13 A man walks along a four-block stretch of Park Avenue (see Figure 11.3). If he is at corner 1, 2, or 3, then he walks to the left or right with equal probability. He continues until he reaches corner 4, which is a bar, or corner 0, which is his home. If he reaches either home or the bar, he stays there.

We form a Markov chain with states 0, 1, 2, 3, and 4. States 0 and 4 are absorbing states. The transition matrix is then

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The states 1, 2, and 3 are transient states, and from any of these it is possible to reach the absorbing states 0 and 4. Hence the chain is an absorbing chain. When a process reaches an absorbing state, we shall say that it is *absorbed*. \Box

The most obvious question that can be asked about such a chain is: What is the probability that the process will eventually reach an absorbing state? Other interesting questions include: (a) What is the probability that the process will end up in a given absorbing state? (b) On the average, how long will it take for the process to be absorbed? (c) On the average, how many times will the process be in each transient state? The answers to all these questions depend, in general, on the state from which the process starts as well as the transition probabilities.

Canonical Form

Consider an arbitrary absorbing Markov chain. Renumber the states so that the transient states come first. If there are r absorbing states and t transient states, the transition matrix will have the following *canonical form*

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$$\mathbf{P} = \frac{\text{TR. ABS.}}{\text{ABS.}} \left(\frac{\mathbf{Q} \quad \mathbf{R}}{\mathbf{0} \quad \mathbf{I}} \right)$$

Here **I** is an *r*-by-*r* identity matrix, **0** is an *r*-by-*t* zero matrix, **R** is a nonzero *t*-by-*r* matrix, and **Q** is an *t*-by-*t* matrix. The first *t* states are transient and the last *r* states are absorbing.

In Section 11.1, we saw that the entry $p_{ij}^{(n)}$ of the matrix \mathbf{P}^n is the probability of being in the state s_j after n steps, when the chain is started in state s_i . A standard matrix algebra argument shows that \mathbf{P}^n is of the form

$$\mathbf{P}^{n} = \frac{\mathrm{TR.}}{\mathrm{ABS.}} \left(\begin{array}{c|c} \mathrm{TR.} & \mathrm{ABS.} \\ \hline \mathbf{Q}^{n} & * \\ \hline \mathbf{0} & \mathbf{I} \end{array} \right)$$

where the asterisk * stands for the *t*-by-*r* matrix in the upper right-hand corner of \mathbf{P}^n . (This submatrix can be written in terms of \mathbf{Q} and \mathbf{R} , but the expression is complicated and is not needed at this time.) The form of \mathbf{P}^n shows that the entries of \mathbf{Q}^n give the probabilities for being in each of the transient states after *n* steps for each possible transient starting state. For our first theorem we prove that the probability of being in the transient states after *n* steps approaches zero. Thus every entry of \mathbf{Q}^n must approach zero as *n* approaches infinity (i.e, $\mathbf{Q}^n \to \mathbf{0}$).

In the following, if **u** and **v** are two vectors we say that $\mathbf{u} \leq \mathbf{v}$ if all components of **u** are less than or equal to the corresponding components of **v**. Similarly, if **A** and **B** are matrices then $\mathbf{A} \leq \mathbf{B}$ if each entry of **A** is less than or equal to the corresponding entry of **B**.

Probability of Absorption

Theorem 11.3 In an absorbing Markov chain, the probability that the process will be absorbed is 1 (i.e., $\mathbf{Q}^n \to \mathbf{0}$ as $n \to \infty$).

Proof. From each nonabsorbing state s_j it is possible to reach an absorbing state. Let m_j be the minimum number of steps required to reach an absorbing state, starting from s_j . Let p_j be the probability that, starting from s_j , the process will not reach an absorbing state in m_j steps. Then $p_j < 1$. Let m be the largest of the m_j and let p be the largest of p_j . The probability of not being absorbed in m steps is less than or equal to p, in 2n steps less than or equal to p^2 , etc. Since p < 1 these probabilities tend to 0. Since the probability of not being absorbed in n steps is monotone decreasing, these probabilities also tend to 0, hence $\lim_{n\to\infty} \mathbf{Q}^n = 0$. \Box

The Fundamental Matrix

Theorem 11.4 For an absorbing Markov chain the matrix $\mathbf{I} - \mathbf{Q}$ has an inverse \mathbf{N} and $\mathbf{N} = \mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \cdots$. The *ij*-entry n_{ij} of the matrix \mathbf{N} is the expected number of times the chain is in state s_j , given that it starts in state s_i . The initial state is counted if i = j.

Proof. Let $(\mathbf{I} - \mathbf{Q})\mathbf{x} = 0$; that is $\mathbf{x} = \mathbf{Q}\mathbf{x}$. Then, iterating this we see that $\mathbf{x} = \mathbf{Q}^n \mathbf{x}$. Since $\mathbf{Q}^n \to \mathbf{0}$, we have $\mathbf{Q}^n \mathbf{x} \to \mathbf{0}$, so $\mathbf{x} = \mathbf{0}$. Thus $(\mathbf{I} - \mathbf{Q})^{-1} = \mathbf{N}$ exists. Note next that

$$(\mathbf{I} - \mathbf{Q})(\mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \dots + \mathbf{Q}^n) = \mathbf{I} - \mathbf{Q}^{n+1}$$
.

Thus multiplying both sides by \mathbf{N} gives

$$\mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \dots + \mathbf{Q}^n = \mathbf{N}(\mathbf{I} - \mathbf{Q}^{n+1})$$
.

Letting n tend to infinity we have

$$\mathbf{N} = \mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \cdots$$

Let s_i and s_j be two transient states, and assume throughout the remainder of the proof that *i* and *j* are fixed. Let $X^{(k)}$ be a random variable which equals 1 if the chain is in state s_j after *k* steps, and equals 0 otherwise. For each *k*, this random variable depends upon both *i* and *j*; we choose not to explicitly show this dependence in the interest of clarity. We have

$$P(X^{(k)} = 1) = q_{ij}^{(k)}$$

and

$$P(X^{(k)} = 0) = 1 - q_{ij}^{(k)}$$
,

where $q_{ij}^{(k)}$ is the *ij*th entry of \mathbf{Q}^k . These equations hold for k = 0 since $\mathbf{Q}^0 = \mathbf{I}$. Therefore, since $X^{(k)}$ is a 0-1 random variable, $E(X^{(k)}) = q_{ij}^{(k)}$.

The expected number of times the chain is in state s_j in the first *n* steps, given that it starts in state s_i , is clearly

$$E\left(X^{(0)} + X^{(1)} + \dots + X^{(n)}\right) = q_{ij}^{(0)} + q_{ij}^{(1)} + \dots + q_{ij}^{(n)}$$

Letting n tend to infinity we have

$$E(X^{(0)} + X^{(1)} + \cdots) = q_{ij}^{(0)} + q_{ij}^{(1)} + \cdots = n_{ij}$$
.

Definition 11.3 For an absorbing Markov chain \mathbf{P} , the matrix $\mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1}$ is called the *fundamental matrix* for \mathbf{P} . The entry n_{ij} of \mathbf{N} gives the expected number of times that the process is in the transient state s_j if it is started in the transient state s_i .

Example 11.14 (Example 11.13 continued) In the Drunkard's Walk example, the transition matrix in canonical form is

$$\mathbf{P} = \frac{1}{4} \begin{pmatrix} 1 & 2 & 3 & 0 & 4 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 2 & 1/2 & 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 \\ \hline 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ \end{pmatrix}$$

From this we see that the matrix \mathbf{Q} is

$$\mathbf{Q} = \begin{pmatrix} 0 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 \end{pmatrix} \ ,$$

and

$$\mathbf{I} - \mathbf{Q} = \begin{pmatrix} 1 & -1/2 & 0\\ -1/2 & 1 & -1/2\\ 0 & -1/2 & 1 \end{pmatrix} \ .$$

Computing $(\mathbf{I} - \mathbf{Q})^{-1}$, we find

$$\mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1} = \begin{array}{ccc} 1 & 2 & 3 \\ 1 & 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 3 & 1/2 & 1 & 3/2 \end{array} \right) \,.$$

From the middle row of N, we see that if we start in state 2, then the expected number of times in states 1, 2, and 3 before being absorbed are 1, 2, and 1. \Box

Time to Absorption

We now consider the question: Given that the chain starts in state s_i , what is the expected number of steps before the chain is absorbed? The answer is given in the next theorem.

Theorem 11.5 Let t_i be the expected number of steps before the chain is absorbed, given that the chain starts in state s_i , and let **t** be the column vector whose *i*th entry is t_i . Then

$$\mathbf{t} = \mathbf{N}\mathbf{c}$$
,

where \mathbf{c} is a column vector all of whose entries are 1.

Proof. If we add all the entries in the *i*th row of \mathbf{N} , we will have the expected number of times in any of the transient states for a given starting state s_i , that is, the expected time required before being absorbed. Thus, t_i is the sum of the entries in the *i*th row of \mathbf{N} . If we write this statement in matrix form, we obtain the theorem. \Box

Absorption Probabilities

Theorem 11.6 Let b_{ij} be the probability that an absorbing chain will be absorbed in the absorbing state s_j if it starts in the transient state s_i . Let **B** be the matrix with entries b_{ij} . Then **B** is an *t*-by-*r* matrix, and

$$\mathbf{B} = \mathbf{NR}$$
.

where \mathbf{N} is the fundamental matrix and \mathbf{R} is as in the canonical form.

Proof. We have

$$\mathbf{B}_{ij} = \sum_{n} \sum_{k} q_{ik}^{(n)} r_{kj}$$
$$= \sum_{k} \sum_{n} q_{ik}^{(n)} r_{kj}$$
$$= \sum_{k} n_{ik} r_{kj}$$
$$= (\mathbf{NR})_{ij} .$$

This completes the proof.

Another proof of this is given in Exercise 34.

Example 11.15 (Example 11.14 continued) In the Drunkard's Walk example, we found that

$$\mathbf{N} = \begin{array}{ccc} 1 & 2 & 3 \\ 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 3 & 1/2 & 1 & 3/2 \end{array} \right) \,.$$

Hence,

$$\mathbf{t} = \mathbf{N}\mathbf{c} = \begin{pmatrix} 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 3/2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$
$$= \begin{pmatrix} 3 \\ 4 \\ 3 \end{pmatrix} .$$

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Thus, starting in states 1, 2, and 3, the expected times to absorption are 3, 4, and 3, respectively.

From the canonical form,

$$\mathbf{R} = \begin{array}{ccc} 0 & 4 \\ 1 & 1/2 & 0 \\ 2 & 0 & 0 \\ 3 & 0 & 1/2 \end{array} \right) \, .$$

Hence,

$$\mathbf{B} = \mathbf{NR} = \begin{pmatrix} 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 3/2 \end{pmatrix} \cdot \begin{pmatrix} 1/2 & 0 \\ 0 & 0 \\ 0 & 1/2 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 4 \\ 1 \\ 2 \\ 3 \\ 1/2 & 1/2 \\ 1/4 & 3/4 \end{pmatrix}.$$

Here the first row tells us that, starting from state 1, there is probability 3/4 of absorption in state 0 and 1/4 of absorption in state 4.

Computation

The fact that we have been able to obtain these three descriptive quantities in matrix form makes it very easy to write a computer program that determines these quantities for a given absorbing chain matrix.

The program **AbsorbingChain** calculates the basic descriptive quantities of an absorbing Markov chain.

We have run the program **AbsorbingChain** for the example of the drunkard's walk (Example 11.13) with 5 blocks. The results are as follows:

$$\mathbf{Q} = \begin{array}{cccc} 1 & 2 & 3 & 4 \\ 1 & (.00 & .50 & .00 & .00 \\ .50 & .00 & .50 & .00 \\ .00 & .50 & .00 & .50 \\ .00 & .00 & .50 & .00 \end{array});$$
$$\mathbf{R} = \begin{array}{c} 0 & 5 \\ 1 & (.50 & .00 \\ .00 & .00 \\ .00 & .00 \\ .00 & .50 \end{array});$$

Note that the probability of reaching the bar before reaching home, starting at x, is x/5 (i.e., proportional to the distance of home from the starting point). (See Exercise 24.)

Exercises

- **1** In Example 11.4, for what values of *a* and *b* do we obtain an absorbing Markov chain?
- 2 Show that Example 11.7 is an absorbing Markov chain.
- **3** Which of the genetics examples (Examples 11.9, 11.10, and 11.11) are absorbing?
- 4 Find the fundamental matrix N for Example 11.10.
- 5 For Example 11.11, verify that the following matrix is the inverse of I Q and hence is the fundamental matrix N.

$$\mathbf{N} = \begin{pmatrix} 8/3 & 1/6 & 4/3 & 2/3 \\ 4/3 & 4/3 & 8/3 & 4/3 \\ 4/3 & 1/3 & 8/3 & 4/3 \\ 2/3 & 1/6 & 4/3 & 8/3 \end{pmatrix} \ .$$

Find \mathbf{Nc} and $\mathbf{NR}.$ Interpret the results.

6 In the Land of Oz example (Example 11.1), change the transition matrix by making R an absorbing state. This gives

$$\mathbf{P} = \begin{array}{ccc} \mathbf{R} & \mathbf{N} & \mathbf{S} \\ \mathbf{P} = \begin{array}{ccc} \mathbf{R} \\ \mathbf{N} \\ \mathbf{S} \end{array} \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} \,.$$

Find the fundamental matrix N, and also Nc and NR. Interpret the results.

- 7 In Example 11.8, make states 0 and 4 into absorbing states. Find the fundamental matrix **N**, and also **Nc** and **NR**, for the resulting absorbing chain. Interpret the results.
- 8 In Example 11.13 (Drunkard's Walk) of this section, assume that the probability of a step to the right is 2/3, and a step to the left is 1/3. Find N, Nc, and NR. Compare these with the results of Example 11.15.
- **9** A process moves on the integers 1, 2, 3, 4, and 5. It starts at 1 and, on each successive step, moves to an integer greater than its present position, moving with equal probability to each of the remaining larger integers. State five is an absorbing state. Find the expected number of steps to reach state five.
- 10 Using the result of Exercise 9, make a conjecture for the form of the fundamental matrix if the process moves as in that exercise, except that it now moves on the integers from 1 to n. Test your conjecture for several different values of n. Can you conjecture an estimate for the expected number of steps to reach state n, for large n? (See Exercise 11 for a method of determining this expected number of steps.)
- *11 Let b_k denote the expected number of steps to reach n from n k, in the process described in Exercise 9.
 - (a) Define $b_0 = 0$. Show that for k > 0, we have

$$b_k = 1 + \frac{1}{k} (b_{k-1} + b_{k-2} + \dots + b_0)$$

(b) Let

$$f(x) = b_0 + b_1 x + b_2 x^2 + \cdots$$

Using the recursion in part (a), show that f(x) satisfies the differential equation

$$(1-x)^2y' - (1-x)y + 1 = 0.$$

(c) Show that the general solution of the differential equation in part (b) is

$$y = \frac{-\log(1-x)}{1-x} + \frac{c}{1-x}$$
,

where c is a constant.

(d) Use part (c) to show that

$$b_k = 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{k}$$
.

12 Three tanks fight a three-way duel. Tank A has probability 1/2 of destroying the tank at which it fires, tank B has probability 1/3 of destroying the tank at which it fires, and tank C has probability 1/6 of destroying the tank at which

it fires. The tanks fire together and each tank fires at the strongest opponent not yet destroyed. Form a Markov chain by taking as states the subsets of the set of tanks. Find **N**, **Nc**, and **NR**, and interpret your results. *Hint*: Take as states ABC, AC, BC, A, B, C, and none, indicating the tanks that could survive starting in state ABC. You can omit AB because this state cannot be reached from ABC.

- 13 Smith is in jail and has 3 dollars; he can get out on bail if he has 8 dollars. A guard agrees to make a series of bets with him. If Smith bets A dollars, he wins A dollars with probability .4 and loses A dollars with probability .6. Find the probability that he wins 8 dollars before losing all of his money if
 - (a) he bets 1 dollar each time (timid strategy).
 - (b) he bets, each time, as much as possible but not more than necessary to bring his fortune up to 8 dollars (bold strategy).
 - (c) Which strategy gives Smith the better chance of getting out of jail?
- 14 With the situation in Exercise 13, consider the strategy such that for i < 4, Smith bets min(i, 4-i), and for $i \ge 4$, he bets according to the bold strategy, where *i* is his current fortune. Find the probability that he gets out of jail using this strategy. How does this probability compare with that obtained for the bold strategy?
- 15 Consider the game of tennis when *deuce* is reached. If a player wins the next point, he has *advantage*. On the following point, he either wins the game or the game returns to *deuce*. Assume that for any point, player A has probability .6 of winning the point and player B has probability .4 of winning the point.
 - (a) Set this up as a Markov chain with state 1: A wins; 2: B wins; 3: advantage A; 4: deuce; 5: advantage B.
 - (b) Find the absorption probabilities.
 - (c) At deuce, find the expected duration of the game and the probability that B will win.

Exercises 16 and 17 concern the inheritance of color-blindness, which is a sexlinked characteristic. There is a pair of genes, g and G, of which the former tends to produce color-blindness, the latter normal vision. The G gene is dominant. But a man has only one gene, and if this is g, he is color-blind. A man inherits one of his mother's two genes, while a woman inherits one gene from each parent. Thus a man may be of type G or g, while a woman may be type GG or Gg or gg. We will study a process of inbreeding similar to that of Example 11.11 by constructing a Markov chain.

16 List the states of the chain. *Hint*: There are six. Compute the transition probabilities. Find the fundamental matrix N, Nc, and NR.

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- 17 Show that in both Example 11.11 and the example just given, the probability of absorption in a state having genes of a particular type is equal to the proportion of genes of that type in the starting state. Show that this can be explained by the fact that a game in which your fortune is the number of genes of a particular type in the state of the Markov chain is a fair game.⁵
- 18 Assume that a student going to a certain four-year medical school in northern New England has, each year, a probability q of flunking out, a probability r of having to repeat the year, and a probability p of moving on to the next year (in the fourth year, moving on means graduating).
 - (a) Form a transition matrix for this process taking as states F, 1, 2, 3, 4, and G where F stands for flunking out and G for graduating, and the other states represent the year of study.
 - (b) For the case q = .1, r = .2, and p = .7 find the time a beginning student can expect to be in the second year. How long should this student expect to be in medical school?
 - (c) Find the probability that this beginning student will graduate.
- 19 (E. Brown⁶) Mary and John are playing the following game: They have a three-card deck marked with the numbers 1, 2, and 3 and a spinner with the numbers 1, 2, and 3 on it. The game begins by dealing the cards out so that the dealer gets one card and the other person gets two. A move in the game consists of a spin of the spinner. The person having the card with the number that comes up on the spinner hands that card to the other person. The game ends when someone has all the cards.
 - (a) Set up the transition matrix for this absorbing Markov chain, where the states correspond to the number of cards that Mary has.
 - (b) Find the fundamental matrix.
 - (c) On the average, how many moves will the game last?
 - (d) If Mary deals, what is the probability that John will win the game?
- 20 Assume that an experiment has m equally probable outcomes. Show that the expected number of independent trials before the first occurrence of k consecutive occurrences of one of these outcomes is $(m^k 1)/(m 1)$. Hint: Form an absorbing Markov chain with states $1, 2, \ldots, k$ with state i representing the length of the current run. The expected time until a run of k is 1 more than the expected time until absorption for the chain started in state 1. It has been found that, in the decimal expansion of pi, starting with the 24,658,601st digit, there is a run of nine 7's. What would your result say about the expected number of digits necessary to find such a run if the digits are produced randomly?

 $^{^5{\}rm H.}$ Gonshor, "An Application of Random Walk to a Problem in Population Genetics," American Math Monthly, vol. 94 (1987), pp. 668–671

⁶Private communication.

- **21** (Roberts⁷) A city is divided into 3 areas 1, 2, and 3. It is estimated that amounts u_1 , u_2 , and u_3 of pollution are emitted each day from these three areas. A fraction q_{ij} of the pollution from region i ends up the next day at region j. A fraction $q_i = 1 \sum_j q_{ij} > 0$ goes into the atmosphere and escapes. Let $w_i^{(n)}$ be the amount of pollution in area i after n days.
 - (a) Show that $\mathbf{w}^{(n)} = \mathbf{u} + \mathbf{u}\mathbf{Q} + \cdots + \mathbf{u}\mathbf{Q}^{n-1}$.
 - (b) Show that $\mathbf{w}^{(n)} \to \mathbf{w}$, and show how to compute \mathbf{w} from \mathbf{u} .
 - (c) The government wants to limit pollution levels to a prescribed level by prescribing \mathbf{w} . Show how to determine the levels of pollution \mathbf{u} which would result in a prescribed limiting value \mathbf{w} .
- **22** In the Leontief economic model,⁸ there are *n* industries 1, 2, ..., *n*. The *i*th industry requires an amount $0 \le q_{ij} \le 1$ of goods (in dollar value) from company *j* to produce 1 dollar's worth of goods. The outside demand on the industries, in dollar value, is given by the vector $\mathbf{d} = (d_1, d_2, \ldots, d_n)$. Let \mathbf{Q} be the matrix with entries q_{ij} .
 - (a) Show that if the industries produce total amounts given by the vector $\mathbf{x} = (x_1, x_2, \dots, x_n)$ then the amounts of goods of each type that the industries will need just to meet their internal demands is given by the vector $\mathbf{x}\mathbf{Q}$.
 - (b) Show that in order to meet the outside demand **d** and the internal demands the industries must produce total amounts given by a vector $\mathbf{x} = (x_1, x_2, \dots, x_n)$ which satisfies the equation $\mathbf{x} = \mathbf{x}\mathbf{Q} + \mathbf{d}$.
 - (c) Show that if **Q** is the **Q**-matrix for an absorbing Markov chain, then it is possible to meet any outside demand **d**.
 - (d) Assume that the row sums of \mathbf{Q} are less than or equal to 1. Give an economic interpretation of this condition. Form a Markov chain by taking the states to be the industries and the transition probabilities to be the q_{ij} . Add one absorbing state 0. Define

$$q_{i0} = 1 - \sum_j q_{ij} \; .$$

Show that this chain will be absorbing if every company is either making a profit or ultimately depends upon a profit-making company.

- (e) Define xc to be the gross national product. Find an expression for the gross national product in terms of the demand vector d and the vector t giving the expected time to absorption.
- **23** A gambler plays a game in which on each play he wins one dollar with probability p and loses one dollar with probability q = 1 p. The *Gambler's Ruin*

⁷F. Roberts, *Discrete Mathematical Models* (Englewood Cliffs, NJ: Prentice Hall, 1976).

⁸W. W. Leontief, Input-Output Economics (Oxford: Oxford University Press, 1966).

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problem is the problem of finding the probability w_x of winning an amount T before losing everything, starting with state x. Show that this problem may be considered to be an absorbing Markov chain with states $0, 1, 2, \ldots, T$ with 0 and T absorbing states. Suppose that a gambler has probability p = .48 of winning on each play. Suppose, in addition, that the gambler starts with 50 dollars and that T = 100 dollars. Simulate this game 100 times and see how often the gambler is ruined. This estimates w_{50} .

24 Show that w_x of Exercise 23 satisfies the following conditions:

- (a) $w_x = pw_{x+1} + qw_{x-1}$ for x = 1, 2, ..., T 1.
- (b) $w_0 = 0$.
- (c) $w_T = 1$.

Show that these conditions determine w_x . Show that, if p = q = 1/2, then

$$w_x = \frac{x}{T}$$

satisfies (a), (b), and (c) and hence is the solution. If $p \neq q$, show that

$$w_x = \frac{(q/p)^x - 1}{(q/p)^T - 1}$$

satisfies these conditions and hence gives the probability of the gambler winning.

- **25** Write a program to compute the probability w_x of Exercise 24 for given values of x, p, and T. Study the probability that the gambler will ruin the bank in a game that is only slightly unfavorable, say p = .49, if the bank has significantly more money than the gambler.
- *26 We considered the two examples of the Drunkard's Walk corresponding to the cases n = 4 and n = 5 blocks (see Example 11.13). Verify that in these two examples the expected time to absorption, starting at x, is equal to x(n x). See if you can prove that this is true in general. *Hint*: Show that if f(x) is the expected time to absorption then f(0) = f(n) = 0 and

$$f(x) = (1/2)f(x-1) + (1/2)f(x+1) + 1$$

for 0 < x < n. Show that if $f_1(x)$ and $f_2(x)$ are two solutions, then their difference g(x) is a solution of the equation

$$g(x) = (1/2)g(x-1) + (1/2)g(x+1)$$
.

Also, g(0) = g(n) = 0. Show that it is not possible for g(x) to have a strict maximum or a strict minimum at the point *i*, where $1 \le i \le n - 1$. Use this to show that g(i) = 0 for all i. This shows that there is at most one solution. Then verify that the function f(x) = x(n-x) is a solution.

27 Consider an absorbing Markov chain with state space S. Let f be a function defined on S with the property that

$$f(i) = \sum_{j \in S} p_{ij} f(j) \; ,$$

or in vector form

$$\mathbf{f}=\mathbf{P}\mathbf{f}$$

Then f is called a *harmonic function* for **P**. If you imagine a game in which your fortune is f(i) when you are in state i, then the harmonic condition means that the game is *fair* in the sense that your expected fortune after one step is the same as it was before the step.

(a) Show that for f harmonic

 $\mathbf{f} = \mathbf{P}^n \mathbf{f}$

for all n.

(b) Show, using (a), that for f harmonic

$$\mathbf{f} = \mathbf{P}^{\infty} \mathbf{f} ,$$

where

$$\mathbf{P}^{\infty} = \lim_{n \to \infty} \mathbf{P}^n = \left(\begin{array}{c|c} \mathbf{0} & \mathbf{B} \\ \hline \mathbf{0} & \mathbf{I} \end{array} \right) \ .$$

(c) Using (b), prove that when you start in a transient state *i* your expected final fortune

$$\sum_{k} b_{ik} f(k)$$

is equal to your starting fortune f(i). In other words, a fair game on a finite state space remains fair to the end. (Fair games in general are called *martingales*. Fair games on infinite state spaces need not remain fair with an unlimited number of plays allowed. For example, consider the game of Heads or Tails (see Example 1.4). Let Peter start with 1 penny and play until he has 2. Then Peter will be sure to end up 1 penny ahead.)

28 A coin is tossed repeatedly. We are interested in finding the expected number of tosses until a particular pattern, say B = HTH, occurs for the first time. If, for example, the outcomes of the tosses are HHTTHTH we say that the pattern B has occurred for the first time after 7 tosses. Let T^B be the time to obtain pattern B for the first time. Li⁹ gives the following method for determining $E(T^B)$.

We are in a casino and, before each toss of the coin, a gambler enters, pays 1 dollar to play, and bets that the pattern B = HTH will occur on the next

⁹S-Y. R. Li, "A Martingale Approach to the Study of Occurrence of Sequence Patterns in Repeated Experiments," *Annals of Probability*, vol. 8 (1980), pp. 1171–1176.

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three tosses. If H occurs, he wins 2 dollars and bets this amount that the next outcome will be T. If he wins, he wins 4 dollars and bets this amount that H will come up next time. If he wins, he wins 8 dollars and the pattern has occurred. If at any time he loses, he leaves with no winnings.

Let A and B be two patterns. Let AB be the amount the gamblers win who arrive while the pattern A occurs and bet that B will occur. For example, if A = HT and B = HTH then AB = 2 + 4 = 6 since the first gambler bet on H and won 2 dollars and then bet on T and won 4 dollars more. The second gambler bet on H and lost. If A = HH and B = HTH, then AB = 2 since the first gambler bet on H and won but then bet on T and lost and the second gambler bet on H and won. If A = B = HTH then AB = BB = 8 + 2 = 10.

Now for each gambler coming in, the casino takes in 1 dollar. Thus the casino takes in T^B dollars. How much does it pay out? The only gamblers who go off with any money are those who arrive during the time the pattern B occurs and they win the amount BB. But since all the bets made are perfectly fair bets, it seems quite intuitive that the expected amount the casino takes in should equal the expected amount that it pays out. That is, $E(T^B) = BB$.

Since we have seen that for B = HTH, BB = 10, the expected time to reach the pattern HTH for the first time is 10. If we had been trying to get the pattern B = HHH, then BB = 8 + 4 + 2 = 14 since all the last three gamblers are paid off in this case. Thus the expected time to get the pattern HHH is 14. To justify this argument, Li used a theorem from the theory of martingales (fair games).

We can obtain these expectations by considering a Markov chain whose states are the possible initial segments of the sequence HTH; these states are HTH, HT, H, and \emptyset , where \emptyset is the empty set. Then, for this example, the transition matrix is

	HTH	HT	Н	Ø	
HTH	/ 1	0	0	0 \	
HT	.5	0	0	.5	
H	0	.5	.5	0	,
ø \	0	0	.5	.5/	

and if B = HTH, $E(T^B)$ is the expected time to absorption for this chain started in state \emptyset .

Show, using the associated Markov chain, that the values $E(T^B) = 10$ and $E(T^B) = 14$ are correct for the expected time to reach the patterns HTH and HHH, respectively.

29 We can use the gambling interpretation given in Exercise 28 to find the expected number of tosses required to reach pattern B when we start with pattern A. To be a meaningful problem, we assume that pattern A does not have pattern B as a subpattern. Let $E_A(T^B)$ be the expected time to reach pattern B starting with pattern A. We use our gambling scheme and assume that the first k coin tosses produced the pattern A. During this time, the gambles

made an amount AB. The total amount the gamblers will have made when the pattern B occurs is BB. Thus, the amount that the gamblers made after the pattern A has occurred is BB - AB. Again by the fair game argument, $E_A(T^B) = BB-AB.$

For example, suppose that we start with pattern A = HT and are trying to get the pattern B = HTH. Then we saw in Exercise 28 that AB = 4 and BB = 10 so $E_A(T^B) = BB-AB = 6$.

Verify that this gambling interpretation leads to the correct answer for all starting states in the examples that you worked in Exercise 28.

30 Here is an elegant method due to Guibas and Odlyzko¹⁰ to obtain the expected time to reach a pattern, say HTH, for the first time. Let f(n) be the number of sequences of length n which do not have the pattern HTH. Let $f_p(n)$ be the number of sequences that have the pattern for the first time after n tosses. To each element of f(n), add the pattern HTH. Then divide the resulting sequences into three subsets: the set where HTH occurs for the first time at time n + 1 (for this, the original sequence must have ended with HT); the set where HTH occurs for the first time at time n + 3 (the original sequence ended with anything except HT). Doing this, we have

$$f(n) = f_p(n+1) + f_p(n+3)$$
.

Thus,

$$\frac{f(n)}{2^n} = \frac{2f_p(n+1)}{2^{n+1}} + \frac{2^3f_p(n+3)}{2^{n+3}} \, .$$

If T is the time that the pattern occurs for the first time, this equality states that

$$P(T > n) = 2P(T = n + 1) + 8P(T = n + 3)$$
.

Show that if you sum this equality over all n you obtain

$$\sum_{n=0}^{\infty} P(T > n) = 2 + 8 = 10 .$$

Show that for any integer-valued random variable

$$E(T) = \sum_{n=0}^{\infty} P(T > n) \; .$$

and conclude that E(T) = 10. Note that this method of proof makes very clear that E(T) is, in general, equal to the expected amount the casino pays out and avoids the martingale system theorem used by Li.

¹⁰L. J. Guibas and A. M. Odlyzko, "String Overlaps, Pattern Matching, and Non-transitive Games," *Journal of Combinatorial Theory*, Series A, vol. 30 (1981), pp. 183–208.

11.2. ABSORBING MARKOV CHAINS

- **31** In Example 11.11, define f(i) to be the proportion of G genes in state *i*. Show that *f* is a harmonic function (see Exercise 27). Why does this show that the probability of being absorbed in state (GG, GG) is equal to the proportion of G genes in the starting state? (See Exercise 17.)
- **32** Show that the stepping stone model (Example 11.12) is an absorbing Markov chain. Assume that you are playing a game with red and green squares, in which your fortune at any time is equal to the proportion of red squares at that time. Give an argument to show that this is a fair game in the sense that your expected winning after each step is just what it was before this step.*Hint*: Show that for every possible outcome in which your fortune will decrease by one there is another outcome of exactly the same probability where it will increase by one.

Use this fact and the results of Exercise 27 to show that the probability that a particular color wins out is equal to the proportion of squares that are initially of this color.

33 Consider a random walker who moves on the integers $0, 1, \ldots, N$, moving one step to the right with probability p and one step to the left with probability q = 1 - p. If the walker ever reaches 0 or N he stays there. (This is the Gambler's Ruin problem of Exercise 23.) If p = q show that the function

f(i) = i

is a harmonic function (see Exercise 27), and if $p \neq q$ then

$$f(i) = \left(\frac{q}{p}\right)^i$$

is a harmonic function. Use this and the result of Exercise 27 to show that the probability b_{iN} of being absorbed in state N starting in state i is

$$b_{iN} = \begin{cases} \frac{i}{N}, & \text{if } p = q, \\ \frac{(\frac{q}{p})^i - 1}{(\frac{q}{p})^N - 1}, & \text{if } p \neq q. \end{cases}$$

For an alternative derivation of these results see Exercise 24.

34 Complete the following alternate proof of Theorem 11.6. Let s_i be a transient state and s_j be an absorbing state. If we compute b_{ij} in terms of the possibilities on the outcome of the first step, then we have the equation

$$b_{ij} = p_{ij} + \sum_k p_{ik} b_{kj} \; ,$$

where the summation is carried out over all transient states s_k . Write this in matrix form, and derive from this equation the statement

$$\mathbf{B} = \mathbf{NR}$$
.

- **35** In Monte Carlo roulette (see Example 6.6), under option (c), there are six states $(S, W, L, E, P_1, \text{ and } P_2)$. The reader is referred to Figure 6.2, which contains a tree for this option. Form a Markov chain for this option, and use the program **AbsorbingChain** to find the probabilities that you win, lose, or break even for a 1 franc bet on red. Using these probabilities, find the expected winnings for this bet. For a more general discussion of Markov chains applied to roulette, see the article of H. Sagan referred to in Example 6.13.
- **36** We consider next a game called *Penney-ante* by its inventor W. Penney.¹¹ There are two players; the first player picks a pattern A of H's and T's, and then the second player, knowing the choice of the first player, picks a different pattern B. We assume that neither pattern is a subpattern of the other pattern. A coin is tossed a sequence of times, and the player whose pattern comes up first is the winner. To analyze the game, we need to find the probability p_A that pattern A will occur before pattern B and the probability $p_B = 1 p_A$ that pattern B occurs before pattern A. To determine these probabilities we use the results of Exercises 28 and 29. Here you were asked to show that, the expected time to reach a pattern B for the first time is,

$$E(T^B) = BB$$

and, starting with pattern A, the expected time to reach pattern B is

$$E_A(T^B) = BB - AB \; .$$

(a) Show that the odds that the first player will win are given by John Conway's formula¹²:

$$\frac{p_A}{1-p_A} = \frac{p_A}{p_B} = \frac{BB-BA}{AA-AB} \; .$$

Hint: Explain why

$$E(T^B) = E(T^A \text{ or } B) + p_A E_A(T^B)$$

and thus

$$BB = E(T^A \text{ or } B) + p_A(BB - AB)$$

Interchange A and B to find a similar equation involving the p_B . Finally, note that

$$p_A + p_B = 1 \; .$$

Use these equations to solve for p_A and p_B .

(b) Assume that both players choose a pattern of the same length k. Show that, if k = 2, this is a fair game, but, if k = 3, the second player has an advantage no matter what choice the first player makes. (It has been shown that, for $k \ge 3$, if the first player chooses a_1, a_2, \ldots, a_k , then the optimal strategy for the second player is of the form b, a_1, \ldots, a_{k-1} where b is the better of the two choices H or T.¹³)

¹¹W. Penney, "Problem: Penney-Ante," Journal of Recreational Math, vol. 2 (1969), p. 241.

¹²M. Gardner, "Mathematical Games," Scientific American, vol. 10 (1974), pp. 120–125.

¹³Guibas and Odlyzko, op. cit.

11.3 Ergodic Markov Chains

A second important kind of Markov chain we shall study in detail is an *ergodic* Markov chain, defined as follows.

Definition 11.4 A Markov chain is called an *ergodic* chain if it is possible to go from every state to every state (not necessarily in one move). \Box

In many books, ergodic Markov chains are called *irreducible*.

Definition 11.5 A Markov chain is called a *regular* chain if some power of the transition matrix has only positive elements. \Box

In other words, for some n, it is possible to go from any state to any state in exactly n steps. It is clear from this definition that every regular chain is ergodic. On the other hand, an ergodic chain is not necessarily regular, as the following examples show.

Example 11.16 Let the transition matrix of a Markov chain be defined by

$$\mathbf{P} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,.$$

Then is clear that it is possible to move from any state to any state, so the chain is ergodic. However, if n is odd, then it is not possible to move from state 0 to state 0 in n steps, and if n is even, then it is not possible to move from state 0 to state 1 in n steps, so the chain is not regular.

A more interesting example of an ergodic, non-regular Markov chain is provided by the Ehrenfest urn model.

Example 11.17 Recall the Ehrenfest urn model (Example 11.8). The transition matrix for this example is

$$\mathbf{P} = \begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1/4 & 0 & 3/4 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 3/4 & 0 & 1/4 \\ 0 & 0 & 0 & 1 & 0 \end{array} \right)$$

In this example, if we start in state 0 we will, after any even number of steps, be in either state 0, 2 or 4, and after any odd number of steps, be in states 1 or 3. Thus this chain is ergodic but not regular. \Box

Regular Markov Chains

Any transition matrix that has no zeros determines a regular Markov chain. However, it is possible for a regular Markov chain to have a transition matrix that has zeros. The transition matrix of the Land of Oz example of Section 11.1 has $p_{NN} = 0$ but the second power \mathbf{P}^2 has no zeros, so this is a regular Markov chain.

An example of a nonregular Markov chain is an absorbing chain. For example, let

$$\mathbf{P} = \begin{pmatrix} 1 & 0\\ 1/2 & 1/2 \end{pmatrix}$$

be the transition matrix of a Markov chain. Then all powers of \mathbf{P} will have a 0 in the upper right-hand corner.

We shall now discuss two important theorems relating to regular chains.

Theorem 11.7 Let **P** be the transition matrix for a regular chain. Then, as $n \to \infty$, the powers \mathbf{P}^n approach a limiting matrix **W** with all rows the same vector **w**. The vector **w** is a strictly positive probability vector (i.e., the components are all positive and they sum to one).

In the next section we give two proofs of this fundamental theorem. We give here the basic idea of the first proof.

We want to show that the powers \mathbf{P}^n of a regular transition matrix tend to a matrix with all rows the same. This is the same as showing that \mathbf{P}^n converges to a matrix with constant columns. Now the *j*th column of \mathbf{P}^n is $\mathbf{P}^n \mathbf{y}$ where \mathbf{y} is a column vector with 1 in the *j*th entry and 0 in the other entries. Thus we need only prove that for any column vector $\mathbf{y}, \mathbf{P}^n \mathbf{y}$ approaches a constant vector as *n* tend to infinity.

Since each row of \mathbf{P} is a probability vector, $\mathbf{P}\mathbf{y}$ replaces \mathbf{y} by averages of its components. Here is an example:

$$\begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/2 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 1/2 \cdot 1 + 1/4 \cdot 2 + 1/4 \cdot 3 \\ 1/3 \cdot 1 + 1/3 \cdot 2 + 1/3 \cdot 3 \\ 1/3 \cdot 1 + 1/2 \cdot 2 + 0 \cdot 3 \end{pmatrix} = \begin{pmatrix} 7/4 \\ 2 \\ 3/2 \end{pmatrix} .$$

The result of the averaging process is to make the components of \mathbf{Py} more similar than those of \mathbf{y} . In particular, the maximum component decreases (from 3 to 2) and the minimum component increases (from 1 to 3/2). Our proof will show that as we do more and more of this averaging to get $\mathbf{P}^n \mathbf{y}$, the difference between the maximum and minimum component will tend to 0 as $n \to \infty$. This means $\mathbf{P}^n \mathbf{y}$ tends to a constant vector. The *ij*th entry of \mathbf{P}^n , $p_{ij}^{(n)}$, is the probability that the process will be in state s_j after *n* steps if it starts in state s_i . If we denote the common row of \mathbf{W} by \mathbf{w} , then Theorem 11.7 states that the probability of being in s_j in the long run is approximately w_j , the *j*th entry of \mathbf{w} , and is independent of the starting state. **Example 11.18** Recall that for the Land of Oz example of Section 11.1, the sixth power of the transition matrix \mathbf{P} is, to three decimal places,

$$\mathbf{P}^{6} = \begin{array}{ccc} \mathrm{R} & \mathrm{N} & \mathrm{S} \\ \mathrm{R} & (.4 & .2 & .4 \\ .4 & .2 & .4 \\ \mathrm{S} & (.4 & .2 & .4 \end{array}) \ .$$

Thus, to this degree of accuracy, the probability of rain six days after a rainy day is the same as the probability of rain six days after a nice day, or six days after a snowy day. Theorem 11.7 predicts that, for large n, the rows of \mathbf{P} approach a common vector. It is interesting that this occurs so soon in our example.

Theorem 11.8 Let P be a regular transition matrix, let

$$\mathbf{W} = \lim_{n \to \infty} \mathbf{P}^n \; ,$$

let \mathbf{w} be the common row of \mathbf{W} , and let \mathbf{c} be the column vector all of whose components are 1. Then

- (a) $\mathbf{wP} = \mathbf{w}$, and any row vector \mathbf{v} such that $\mathbf{vP} = \mathbf{v}$ is a constant multiple of \mathbf{w} .
- (b) $\mathbf{Pc} = \mathbf{c}$, and any column vector \mathbf{x} such that $\mathbf{Px} = \mathbf{x}$ is a multiple of \mathbf{c} .

Proof. To prove part (a), we note that from Theorem 11.7,

$$\mathbf{P}^n \to \mathbf{W}$$

Thus,

$$\mathbf{P}^{n+1} = \mathbf{P}^n \cdot \mathbf{P} \to \mathbf{WP}$$

But $\mathbf{P}^{n+1} \to \mathbf{W}$, and so $\mathbf{W} = \mathbf{W}\mathbf{P}$, and $\mathbf{w} = \mathbf{w}\mathbf{P}$.

Let \mathbf{v} be any vector with $\mathbf{vP} = \mathbf{v}$. Then $\mathbf{v} = \mathbf{vP}^n$, and passing to the limit, $\mathbf{v} = \mathbf{vW}$. Let r be the sum of the components of \mathbf{v} . Then it is easily checked that $\mathbf{vW} = r\mathbf{w}$. So, $\mathbf{v} = r\mathbf{w}$.

To prove part (b), assume that $\mathbf{x} = \mathbf{P}\mathbf{x}$. Then $\mathbf{x} = \mathbf{P}^n \mathbf{x}$, and again passing to the limit, $\mathbf{x} = \mathbf{W}\mathbf{x}$. Since all rows of \mathbf{W} are the same, the components of $\mathbf{W}\mathbf{x}$ are all equal, so \mathbf{x} is a multiple of \mathbf{c} .

Note that an immediate consequence of Theorem 11.8 is the fact that there is only one probability vector \mathbf{v} such that $\mathbf{vP} = \mathbf{v}$.

Fixed Vectors

Definition 11.6 A row vector \mathbf{w} with the property $\mathbf{wP} = \mathbf{w}$ is called a *fixed row* vector for \mathbf{P} . Similarly, a column vector \mathbf{x} such that $\mathbf{Px} = \mathbf{x}$ is called a *fixed column* vector for \mathbf{P} .

Thus, the common row of \mathbf{W} is the unique vector \mathbf{w} which is both a fixed row vector for \mathbf{P} and a probability vector. Theorem 11.8 shows that any fixed row vector for \mathbf{P} is a multiple of \mathbf{w} and any fixed column vector for \mathbf{P} is a constant vector.

One can also state Definition 11.6 in terms of eigenvalues and eigenvectors. A fixed row vector is a left eigenvector of the matrix \mathbf{P} corresponding to the eigenvalue 1. A similar statement can be made about fixed column vectors.

We will now give several different methods for calculating the fixed row vector \mathbf{w} for a regular Markov chain.

Example 11.19 By Theorem 11.7 we can find the limiting vector \mathbf{w} for the Land of Oz from the fact that

$$w_1 + w_2 + w_3 = 1$$

and

$$(w_1 \quad w_2 \quad w_3) \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} = (w_1 \quad w_2 \quad w_3) .$$

These relations lead to the following four equations in three unknowns:

$$w_1 + w_2 + w_3 = 1 ,$$

$$(1/2)w_1 + (1/2)w_2 + (1/4)w_3 = w_1 ,$$

$$(1/4)w_1 + (1/4)w_3 = w_2 ,$$

$$(1/4)w_1 + (1/2)w_2 + (1/2)w_3 = w_3 .$$

Our theorem guarantees that these equations have a unique solution. If the equations are solved, we obtain the solution

$$\mathbf{w} = (.4 \quad .2 \quad .4) \quad ,$$

in agreement with that predicted from \mathbf{P}^6 , given in Example 11.2.

To calculate the fixed vector, we can assume that the value at a particular state, say state one, is 1, and then use all but one of the linear equations from $\mathbf{wP} = \mathbf{w}$. This set of equations will have a unique solution and we can obtain \mathbf{w} from this solution by dividing each of its entries by their sum to give the probability vector \mathbf{w} . We will now illustrate this idea for the above example.

Example 11.20 (Example 11.19 continued) We set $w_1 = 1$, and then solve the first and second linear equations from $\mathbf{wP} = \mathbf{w}$. We have

$$(1/2) + (1/2)w_2 + (1/4)w_3 = 1$$
,
 $(1/4) + (1/4)w_3 = w_2$.

If we solve these, we obtain

$$(w_1 \ w_2 \ w_3) = (1 \ 1/2 \ 1)$$
.

Now we divide this vector by the sum of the components, to obtain the final answer:

$$\mathbf{w} = (.4 \ .2 \ .4)$$

This method can be easily programmed to run on a computer.

As mentioned above, we can also think of the fixed row vector \mathbf{w} as a left eigenvector of the transition matrix \mathbf{P} . Thus, if we write \mathbf{I} to denote the identity matrix, then \mathbf{w} satisfies the matrix equation

$$\mathbf{wP} = \mathbf{wI}$$
,

or equivalently,

$$\mathbf{w}(\mathbf{P}-\mathbf{I})=\mathbf{0} \ .$$

Thus, **w** is in the left nullspace of the matrix $\mathbf{P} - \mathbf{I}$. Furthermore, Theorem 11.8 states that this left nullspace has dimension 1. Certain computer programming languages can find nullspaces of matrices. In such languages, one can find the fixed row probability vector for a matrix \mathbf{P} by computing the left nullspace and then normalizing a vector in the nullspace so the sum of its components is 1.

The program **FixedVector** uses one of the above methods (depending upon the language in which it is written) to calculate the fixed row probability vector for regular Markov chains.

So far we have always assumed that we started in a specific state. The following theorem generalizes Theorem 11.7 to the case where the starting state is itself determined by a probability vector.

Theorem 11.9 Let \mathbf{P} be the transition matrix for a regular chain and \mathbf{v} an arbitrary probability vector. Then

$$\lim_{n\to\infty}\mathbf{v}\mathbf{P}^n=\mathbf{w}\;,$$

where \mathbf{w} is the unique fixed probability vector for \mathbf{P} .

Proof. By Theorem 11.7,

$$\lim_{n\to\infty}\mathbf{P}^n=\mathbf{W}\;.$$

Hence,

$$\lim_{n\to\infty}\mathbf{v}\mathbf{P}^n=\mathbf{v}\mathbf{W}$$

But the entries in \mathbf{v} sum to 1, and each row of \mathbf{W} equals \mathbf{w} . From these statements, it is easy to check that

$$\mathbf{v}\mathbf{W} = \mathbf{w}$$
 .

If we start a Markov chain with initial probabilities given by \mathbf{v} , then the probability vector \mathbf{vP}^n gives the probabilities of being in the various states after *n* steps. Theorem 11.9 then establishes the fact that, even in this more general class of processes, the probability of being in s_j approaches w_j .

Equilibrium

We also obtain a new interpretation for \mathbf{w} . Suppose that our starting vector picks state s_i as a starting state with probability w_i , for all i. Then the probability of being in the various states after n steps is given by $\mathbf{wP}^n = \mathbf{w}$, and is the same on all steps. This method of starting provides us with a process that is called "stationary." The fact that \mathbf{w} is the only probability vector for which $\mathbf{wP} = \mathbf{w}$ shows that we must have a starting probability vector of exactly the kind described to obtain a stationary process.

Many interesting results concerning regular Markov chains depend only on the fact that the chain has a unique fixed probability vector which is positive. This property holds for all ergodic Markov chains.

Theorem 11.10 For an ergodic Markov chain, there is a unique probability vector \mathbf{w} such that $\mathbf{wP} = \mathbf{w}$ and \mathbf{w} is strictly positive. Any row vector such that $\mathbf{vP} = \mathbf{v}$ is a multiple of \mathbf{w} . Any column vector \mathbf{x} such that $\mathbf{Px} = \mathbf{x}$ is a constant vector.

Proof. This theorem states that Theorem 11.8 is true for ergodic chains. The result follows easily from the fact that, if **P** is an ergodic transition matrix, then $\bar{\mathbf{P}} = (1/2)\mathbf{I} + (1/2)\mathbf{P}$ is a regular transition matrix with the same fixed vectors (see Exercises 25–28).

For ergodic chains, the fixed probability vector has a slightly different interpretation. The following two theorems, which we will not prove here, furnish an interpretation for this fixed vector.

Theorem 11.11 Let **P** be the transition matrix for an ergodic chain. Let \mathbf{A}_n be the matrix defined by

$$\mathbf{A}_n = \frac{\mathbf{I} + \mathbf{P} + \mathbf{P}^2 + \dots + \mathbf{P}^n}{n+1}$$

Then $\mathbf{A}_n \to \mathbf{W}$, where \mathbf{W} is a matrix all of whose rows are equal to the unique fixed probability vector \mathbf{w} for \mathbf{P} .

If \mathbf{P} is the transition matrix of an ergodic chain, then Theorem 11.8 states that there is only one fixed row probability vector for \mathbf{P} . Thus, we can use the same techniques that were used for regular chains to solve for this fixed vector. In particular, the program **FixedVector** works for ergodic chains.

To interpret Theorem 11.11, let us assume that we have an ergodic chain that starts in state s_i . Let $X^{(m)} = 1$ if the *m*th step is to state s_j and 0 otherwise. Then the average number of times in state s_j in the first *n* steps is given by

$$H^{(n)} = \frac{X^{(0)} + X^{(1)} + X^{(2)} + \dots + X^{(n)}}{n+1}$$

But $X^{(m)}$ takes on the value 1 with probability $p_{ij}^{(m)}$ and 0 otherwise. Thus $E(X^{(m)}) = p_{ij}^{(m)}$, and the *ij*th entry of \mathbf{A}_n gives the expected value of $H^{(n)}$, that

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is, the expected proportion of times in state s_j in the first n steps if the chain starts in state s_i .

If we call being in state s_j success and any other state failure, we could ask if a theorem analogous to the law of large numbers for independent trials holds. The answer is yes and is given by the following theorem.

Theorem 11.12 (Law of Large Numbers for Ergodic Markov Chains) Let $H_j^{(n)}$ be the proportion of times in n steps that an ergodic chain is in state s_j . Then for any $\epsilon > 0$,

$$P\Big(|H_j^{(n)} - w_j| > \epsilon\Big) \to 0 ,$$

independent of the starting state s_i .

We have observed that every regular Markov chain is also an ergodic chain. Hence, Theorems 11.11 and 11.12 apply also for regular chains. For example, this gives us a new interpretation for the fixed vector $\mathbf{w} = (.4, .2, .4)$ in the Land of Oz example. Theorem 11.11 predicts that, in the long run, it will rain 40 percent of the time in the Land of Oz, be nice 20 percent of the time, and snow 40 percent of the time.

Simulation

We illustrate Theorem 11.12 by writing a program to simulate the behavior of a Markov chain. **SimulateChain** is such a program.

Example 11.21 In the Land of Oz, there are 525 days in a year. We have simulated the weather for one year in the Land of Oz, using the program **SimulateChain**. The results are shown in Table 11.2.

State	Times	Fraction
R	217	.413
Ν	109	.208
S	199	.379

Table 11.2: Weather in the Land of Oz.

We note that the simulation gives a proportion of times in each of the states not too different from the long run predictions of .4, .2, and .4 assured by Theorem 11.7. To get better results we have to simulate our chain for a longer time. We do this for 10,000 days without printing out each day's weather. The results are shown in Table 11.3. We see that the results are now quite close to the theoretical values of .4, .2, and .4.

State	Times	Fraction
R	4010	.401
Ν	1902	.19
S	4088	.409

Table 11.3: Comparison of observed and predicted frequencies for the Land of Oz.

Examples of Ergodic Chains

The computation of the fixed vector \mathbf{w} may be difficult if the transition matrix is very large. It is sometimes useful to guess the fixed vector on purely intuitive grounds. Here is a simple example to illustrate this kind of situation.

Example 11.22 A white rat is put into the maze of Figure 11.4. There are nine compartments with connections between the compartments as indicated. The rat moves through the compartments at random. That is, if there are k ways to leave a compartment, it chooses each of these with equal probability. We can represent the travels of the rat by a Markov chain process with transition matrix given by

	1	2	3	4	5	6	7	8	9	
1	(0	1/2	0	0	0	1/2	0	0	0)	
2	1/3	0	1/3	0	1/3	0	0	0	0	
3	0	1/2	0	1/2	0	0	0	0	0	
4	0	0	1/3	0	1/3	0	0	0	1/3	
$\mathbf{P} = 5$	0	1/4	0	1/4	0	1/4	0	1/4	0	.
6	1/3	0	0	0	1/3	0	1/3	0	0	
7	0	0	0	0	0	1/2	0	1/2	0	
8	0	0	0	0	1/3	0	1/3	0	1/3	
9	0	0	0	1/2	0	0	0	1/2	0 /	

That this chain is not regular can be seen as follows: From an odd-numbered state the process can go only to an even-numbered state, and from an even-numbered state it can go only to an odd number. Hence, starting in state i the process will be alternately in even-numbered and odd-numbered states. Therefore, odd powers of **P** will have 0's for the odd-numbered entries in row 1. On the other hand, a glance at the maze shows that it is possible to go from every state to every other state, so that the chain is ergodic.



Figure 11.4: The maze problem.

To find the fixed probability vector for this matrix, we would have to solve ten equations in nine unknowns. However, it would seem reasonable that the times spent in each compartment should, in the long run, be proportional to the number of entries to each compartment. Thus, we try the vector whose jth component is the number of entries to the jth compartment:

$$\mathbf{x} = (2 \ 3 \ 2 \ 3 \ 4 \ 3 \ 2 \ 3 \ 2)$$

It is easy to check that this vector is indeed a fixed vector so that the unique probability vector is this vector normalized to have sum 1:

$$\mathbf{w} = \begin{pmatrix} \frac{1}{12} & \frac{1}{8} & \frac{1}{12} & \frac{1}{8} & \frac{1}{6} & \frac{1}{8} & \frac{1}{12} & \frac{1}{8} & \frac{1}{12} \end{pmatrix} .$$

Example 11.23 (Example 11.8 continued) We recall the Ehrenfest urn model of Example 11.8. The transition matrix for this chain is as follows:

If we run the program **FixedVector** for this chain, we obtain the vector

By Theorem 11.12, we can interpret these values for w_i as the proportion of times the process is in each of the states in the long run. For example, the proportion of times in state 0 is .0625 and the proportion of times in state 1 is .375. The astute reader will note that these numbers are the binomial distribution 1/16, 4/16, 6/16, 4/16, 1/16. We could have guessed this answer as follows: If we consider a particular ball, it simply moves randomly back and forth between the two urns. This suggests that the equilibrium state should be just as if we randomly distributed the four balls in the two urns. If we did this, the probability that there would be exactly j balls in one urn would be given by the binomial distribution b(n, p, j) with n = 4 and p = 1/2.

Exercises

1 Which of the following matrices are transition matrices for regular Markov chains?

(a)
$$\mathbf{P} = \begin{pmatrix} .5 & .5 \\ .5 & .5 \end{pmatrix}$$
.
(b) $\mathbf{P} = \begin{pmatrix} .5 & .5 \\ 1 & 0 \end{pmatrix}$.
(c) $\mathbf{P} = \begin{pmatrix} 1/3 & 0 & 2/3 \\ 0 & 1 & 0 \\ 0 & 1/5 & 4/5 \end{pmatrix}$.
(d) $\mathbf{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.
(e) $\mathbf{P} = \begin{pmatrix} 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$.

 ${\bf 2}\,$ Consider the Markov chain with transition matrix

$$\mathbf{P} = \begin{pmatrix} 1/2 & 1/3 & 1/6 \\ 3/4 & 0 & 1/4 \\ 0 & 1 & 0 \end{pmatrix} \ .$$

- (a) Show that this is a regular Markov chain.
- (b) The process is started in state 1; find the probability that it is in state 3 after two steps.
- (c) Find the limiting probability vector **w**.
- **3** Consider the Markov chain with general 2×2 transition matrix

$$\mathbf{P} = \begin{pmatrix} 1-a & a \\ b & 1-b \end{pmatrix} \ .$$

- (a) Under what conditions is **P** absorbing?
- (b) Under what conditions is **P** ergodic but not regular?
- (c) Under what conditions is **P** regular?

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- **4** Find the fixed probability vector \mathbf{w} for the matrices in Exercise 3 that are ergodic.
- $\mathbf{5}$ Find the fixed probability vector \mathbf{w} for each of the following regular matrices.

(a)
$$\mathbf{P} = \begin{pmatrix} .75 & .25 \\ .5 & .5 \end{pmatrix}$$
.
(b) $\mathbf{P} = \begin{pmatrix} .9 & .1 \\ .1 & .9 \end{pmatrix}$.
(c) $\mathbf{P} = \begin{pmatrix} 3/4 & 1/4 & 0 \\ 0 & 2/3 & 1/3 \\ 1/4 & 1/4 & 1/2 \end{pmatrix}$

6 Consider the Markov chain with transition matrix in Exercise 3, with a = b = 1. Show that this chain is ergodic but not regular. Find the fixed probability vector and interpret it. Show that \mathbf{P}^n does not tend to a limit, but that

$$\mathbf{A}_n = \frac{\mathbf{I} + \mathbf{P} + \mathbf{P}^2 + \dots + \mathbf{P}^n}{n+1}$$

does.

- 7 Consider the Markov chain with transition matrix of Exercise 3, with a = 0 and b = 1/2. Compute directly the unique fixed probability vector, and use your result to prove that the chain is not ergodic.
- 8 Show that the matrix

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0\\ 1/4 & 1/2 & 1/4\\ 0 & 0 & 1 \end{pmatrix}$$

has more than one fixed probability vector. Find the matrix that \mathbf{P}^n approaches as $n \to \infty$, and verify that it is not a matrix all of whose rows are the same.

- **9** Prove that, if a 3-by-3 transition matrix has the property that its *column* sums are 1, then (1/3, 1/3, 1/3) is a fixed probability vector. State a similar result for *n*-by-*n* transition matrices. Interpret these results for ergodic chains.
- 10 Is the Markov chain in Example 11.10 ergodic?
- 11 Is the Markov chain in Example 11.11 ergodic?
- 12 Consider Example 11.13 (Drunkard's Walk). Assume that if the walker reaches state 0, he turns around and returns to state 1 on the next step and, similarly, if he reaches 4 he returns on the next step to state 3. Is this new chain ergodic? Is it regular?
- 13 For Example 11.4 when **P** is ergodic, what is the proportion of people who are told that the President will run? Interpret the fact that this proportion is independent of the starting state.

- 14 Consider an independent trials process to be a Markov chain whose states are the possible outcomes of the individual trials. What is its fixed probability vector? Is the chain always regular? Illustrate this for Example 11.5.
- 15 Show that Example 11.8 is an ergodic chain, but not a regular chain. Show that its fixed probability vector \mathbf{w} is a binomial distribution.
- 16 Show that Example 11.9 is regular and find the limiting vector.
- 17 Toss a fair die repeatedly. Let S_n denote the total of the outcomes through the *n*th toss. Show that there is a limiting value for the proportion of the first *n* values of S_n that are divisible by 7, and compute the value for this limit. *Hint*: The desired limit is an equilibrium probability vector for an appropriate seven state Markov chain.
- 18 Let **P** be the transition matrix of a regular Markov chain. Assume that there are r states and let N(r) be the smallest integer n such that **P** is regular if and only if $\mathbf{P}^{N(r)}$ has no zero entries. Find a finite upper bound for N(r). See if you can determine N(3) exactly.
- *19 Define f(r) to be the smallest integer *n* such that for all regular Markov chains with *r* states, the *n*th power of the transition matrix has all entries positive. It has been shown,¹⁴ that $f(r) = r^2 2r + 2$.
 - (a) Define the transition matrix of an *r*-state Markov chain as follows: For states s_i , with i = 1, 2, ..., r-2, $\mathbf{P}(i, i+1) = 1$, $\mathbf{P}(r-1, r) = \mathbf{P}(r-1, 1) = 1/2$, and $\mathbf{P}(r, 1) = 1$. Show that this is a regular Markov chain.
 - (b) For r = 3, verify that the fifth power is the first power that has no zeros.
 - (c) Show that, for general r, the smallest n such that \mathbf{P}^n has all entries positive is n = f(r).
- **20** A discrete time queueing system of capacity n consists of the person being served and those waiting to be served. The queue length x is observed each second. If 0 < x < n, then with probability p, the queue size is increased by one by an arrival and, inependently, with probability r, it is decreased by one because the person being served finishes service. If x = 0, only an arrival (with probability p) is possible. If x = n, an arrival will depart without waiting for service, and so only the departure (with probability r) of the person being served is possible. Form a Markov chain with states given by the number of customers in the queue. Modify the program **FixedVector** so that you can input n, p, and r, and the program will construct the transition matrix and compute the fixed vector. The quantity s = p/r is called the *traffic intensity*. Describe the differences in the fixed vectors according as s < 1, s = 1, or s > 1.

¹⁴E. Seneta, Non-Negative Matrices: An Introduction to Theory and Applications, Wiley, New York, 1973, pp. 52-54.

11.3. ERGODIC MARKOV CHAINS

- **21** Write a computer program to simulate the queue in Exercise 20. Have your program keep track of the proportion of the time that the queue length is j for j = 0, 1, ..., n and the average queue length. Show that the behavior of the queue length is very different depending upon whether the traffic intensity s has the property s < 1, s = 1, or s > 1.
- **22** In the queueing problem of Exercise 20, let S be the total service time required by a customer and T the time between arrivals of the customers.
 - (a) Show that $P(S = j) = (1 r)^{j-1}r$ and $P(T = j) = (1 p)^{j-1}p$, for j > 0.
 - (b) Show that E(S) = 1/r and E(T) = 1/p.
 - (c) Interpret the conditions s < 1, s = 1 and s > 1 in terms of these expected values.
- 23 In Exercise 20 the service time S has a geometric distribution with E(S) = 1/r. Assume that the service time is, instead, a constant time of t seconds. Modify your computer program of Exercise 21 so that it simulates a constant time service distribution. Compare the average queue length for the two types of distributions when they have the same expected service time (i.e., take t = 1/r). Which distribution leads to the longer queues on the average?
- 24 A certain experiment is believed to be described by a two-state Markov chain with the transition matrix **P**, where

$$\mathbf{P} = \begin{pmatrix} .5 & .5\\ p & 1-p \end{pmatrix}$$

and the parameter p is not known. When the experiment is performed many times, the chain ends in state one approximately 20 percent of the time and in state two approximately 80 percent of the time. Compute a sensible estimate for the unknown parameter p and explain how you found it.

- **25** Prove that, in an *r*-state ergodic chain, it is possible to go from any state to any other state in at most r 1 steps.
- **26** Let **P** be the transition matrix of an *r*-state ergodic chain. Prove that, if the diagonal entries p_{ii} are positive, then the chain is regular.
- 27 Prove that if **P** is the transition matrix of an ergodic chain, then $(1/2)(\mathbf{I} + \mathbf{P})$ is the transition matrix of a regular chain. *Hint*: Use Exercise 26.
- **28** Prove that **P** and $(1/2)(\mathbf{I} + \mathbf{P})$ have the same fixed vectors.
- **29** In his book, *Wahrscheinlichkeitsrechnung und Statistik*,¹⁵ A. Engle proposes an algorithm for finding the fixed vector for an ergodic Markov chain when the transition probabilities are rational numbers. Here is his algorithm: For

¹⁵A. Engle, Wahrscheinlichkeitsrechnung und Statistik, vol. 2 (Stuttgart: Klett Verlag, 1976).

(4	2	4)
(5	2	3)
(8	2	4)
(7	3	4)
(8	4	4)
(8	3	5)
(8	4	8)
(10)	4	6)
(12)	4	8)
(12)	5	7)
(12)	6	8)
(13)	5	8)
(16)	6	8)
(15)	6	9)
(16)	6	12)
(17)	7	10)
(20)	8	12)
(20)	8	12) .

Table 11.4: Distribution of chips.

each state i, let a_i be the least common multiple of the denominators of the non-zero entries in the *i*th row. Engle describes his algorithm in terms of moving chips around on the states—indeed, for small examples, he recommends implementing the algorithm this way. Start by putting a_i chips on state *i* for all *i*. Then, at each state, redistribute the a_i chips, sending $a_i p_{ij}$ to state *j*. The number of chips at state *i* after this redistribution need not be a multiple of a_i . For each state *i*, add just enough chips to bring the number of chips at state *i* after the redistribute the chips in the same manner. This process will eventually reach a point where the number of chips at each state, after the redistribution, is the same as before redistribution. At this point, we have found a fixed vector. Here is an example:

$$\mathbf{P} = \begin{array}{ccc} 1 & 2 & 3 \\ 1 & 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 3 & 1/2 & 1/4 & 1/4 \end{array} \right) \,.$$

We start with $\mathbf{a} = (4, 2, 4)$. The chips after successive redistributions are shown in Table 11.4.

We find that $\mathbf{a} = (20, 8, 12)$ is a fixed vector.

- (a) Write a computer program to implement this algorithm.
- (b) Prove that the algorithm will stop. *Hint*: Let **b** be a vector with integer components that is a fixed vector for **P** and such that each coordinate of

the starting vector \mathbf{a} is less than or equal to the corresponding component of \mathbf{b} . Show that, in the iteration, the components of the vectors are always increasing, and always less than or equal to the corresponding component of \mathbf{b} .

- **30** (Coffman, Kaduta, and Shepp¹⁶) A computing center keeps information on a tape in positions of unit length. During each time unit there is one request to occupy a unit of tape. When this arrives the first free unit is used. Also, during each second, each of the units that are occupied is vacated with probability p. Simulate this process, starting with an empty tape. Estimate the expected number of sites occupied for a given value of p. If p is small, can you choose the tape long enough so that there is a small probability that a new job will have to be turned away (i.e., that all the sites are occupied)? Form a Markov chain with states the number of sites occupied. Modify the program **FixedVector** to compute the fixed vector. Use this to check your conjecture by simulation.
- *31 (Alternate proof of Theorem 11.8) Let **P** be the transition matrix of an ergodic Markov chain. Let **x** be any column vector such that $\mathbf{Px} = \mathbf{x}$. Let M be the maximum value of the components of **x**. Assume that $x_i = M$. Show that if $p_{ij} > 0$ then $x_j = M$. Use this to prove that **x** must be a constant vector.
- **32** Let **P** be the transition matrix of an ergodic Markov chain. Let **w** be a fixed probability vector (i.e., **w** is a row vector with $\mathbf{wP} = \mathbf{w}$). Show that if $w_i = 0$ and $p_{ji} > 0$ then $w_j = 0$. Use this to show that the fixed probability vector for an ergodic chain cannot have any 0 entries.
- 33 Find a Markov chain that is neither absorbing or ergodic.

11.4 Fundamental Limit Theorem for Regular Chains

The fundamental limit theorem for regular Markov chains states that if \mathbf{P} is a regular transition matrix then

$$\lim_{n\to\infty}\mathbf{P}^n=\mathbf{W}\;,$$

where \mathbf{W} is a matrix with each row equal to the unique fixed probability row vector \mathbf{w} for \mathbf{P} . In this section we shall give two very different proofs of this theorem.

Our first proof is carried out by showing that, for any column vector \mathbf{y} , $\mathbf{P}^n \mathbf{y}$ tends to a constant vector. As indicated in Section 11.3, this will show that \mathbf{P}^n converges to a matrix with constant columns or, equivalently, to a matrix with all rows the same.

The following lemma says that if an r-by-r transition matrix has no zero entries, and **y** is any column vector with r entries, then the vector **Py** has entries which are "closer together" than the entries are in **y**.

¹⁶E. G. Coffman, J. T. Kaduta, and L. A. Shepp, "On the Asymptotic Optimality of First-Storage Allocation," *IEEE Trans. Software Engineering*, vol. II (1985), pp. 235-239.

Lemma 11.1 Let **P** be an *r*-by-*r* transition matrix with no zero entries. Let *d* be the smallest entry of the matrix. Let **y** be a column vector with *r* components, the largest of which is M_0 and the smallest m_0 . Let M_1 and m_1 be the largest and smallest component, respectively, of the vector **Py**. Then

$$M_1 - m_1 \le (1 - 2d)(M_0 - m_0)$$
.

Proof. In the discussion following Theorem11.7, it was noted that each entry in the vector \mathbf{Py} is a weighted average of the entries in \mathbf{y} . The largest weighted average that could be obtained in the present case would occur if all but one of the entries of \mathbf{y} have value M_0 and one entry has value m_0 , and this one small entry is weighted by the smallest possible weight, namely d. In this case, the weighted average would equal

$$dm_0 + (1-d)M_0$$
.

Similarly, the smallest possible weighted average equals

$$dM_0 + (1-d)m_0$$
.

Thus,

$$M_1 - m_1 \leq \left(dm_0 + (1-d)M_0 \right) - \left(dM_0 + (1-d)m_0 \right)$$

= $(1-2d)(M_0 - m_0)$.

This completes the proof of the lemma.

We turn now to the proof of the fundamental limit theorem for regular Markov chains.

Theorem 11.13 (Fundamental Limit Theorem for Regular Chains) If **P** is the transition matrix for a regular Markov chain, then

$$\lim_{n\to\infty}\mathbf{P}^n=\mathbf{W}\;,$$

where \mathbf{W} is matrix with all rows equal. Furthermore, all entries in \mathbf{W} are strictly positive.

Proof. We prove this theorem for the special case that \mathbf{P} has no 0 entries. The extension to the general case is indicated in Exercise 5. Let \mathbf{y} be any *r*-component column vector, where r is the number of states of the chain. We assume that r > 1, since otherwise the theorem is trivial. Let M_n and m_n be, respectively, the maximum and minimum components of the vector $\mathbf{P}^n \mathbf{y}$. The vector $\mathbf{P}^n \mathbf{y}$ is obtained from the vector $\mathbf{P}^{n-1}\mathbf{y}$ by multiplying on the left by the matrix \mathbf{P} . Hence each component of $\mathbf{P}^n \mathbf{y}$ is an average of the components of $\mathbf{P}^{n-1}\mathbf{y}$. Thus

$$M_0 \ge M_1 \ge M_2 \ge \cdots$$

and

$$n_0 \leq m_1 \leq m_2 \leq \cdots$$
.

Each sequence is monotone and bounded:

$$m_0 \leq m_n \leq M_n \leq M_0$$
.

Hence, each of these sequences will have a limit as n tends to infinity.

γ

Let M be the limit of M_n and m the limit of m_n . We know that $m \leq M$. We shall prove that M - m = 0. This will be the case if $M_n - m_n$ tends to 0. Let d be the smallest element of **P**. Since all entries of **P** are strictly positive, we have d > 0. By our lemma

$$M_n - m_n \le (1 - 2d)(M_{n-1} - m_{n-1})$$
.

From this we see that

$$M_n - m_n \le (1 - 2d)^n (M_0 - m_0)$$

Since $r \ge 2$, we must have $d \le 1/2$, so $0 \le 1 - 2d < 1$, so the difference $M_n - m_n$ tends to 0 as *n* tends to infinity. Since every component of $\mathbf{P}^n \mathbf{y}$ lies between m_n and M_n , each component must approach the same number u = M = m. This shows that

$$\lim_{n\to\infty}\mathbf{P}^n\mathbf{y}=\mathbf{u}\;,$$

where \mathbf{u} is a column vector all of whose components equal u.

Now let \mathbf{y} be the vector with *j*th component equal to 1 and all other components equal to 0. Then $\mathbf{P}^n \mathbf{y}$ is the *j*th column of \mathbf{P}^n . Doing this for each *j* proves that the columns of \mathbf{P}^n approach constant column vectors. That is, the rows of \mathbf{P}^n approach a common row vector \mathbf{w} , or,

$$\lim_{n\to\infty}\mathbf{P}^n=\mathbf{W}$$

It remains to show that all entries in \mathbf{W} are strictly positive. As before, let \mathbf{y} be the vector with *j*th component equal to 1 and all other components equal to 0. Then $\mathbf{P}\mathbf{y}$ is the *j*th column of \mathbf{P} , and this column has all entries strictly positive. The minimum component of the vector $\mathbf{P}\mathbf{y}$ was defined to be m_1 , hence $m_1 > 0$. Since $m_1 \leq m$, we have m > 0. Note finally that this value of m is just the *j*th component of \mathbf{w} , so all components of \mathbf{w} are strictly positive. \Box

Doeblin's Proof

We give now a very different proof of the main part of the fundamental limit theorem for regular Markov chains. This proof was first given by Doeblin,¹⁷ a brilliant young mathematician who was killed in his twenties in the Second World War.

¹⁷W. Doeblin, "Exposé de la Théorie des Chaines Simple Constantes de Markov à un Nombre Fini d'Etats," *Rev. Mach. de l'Union Interbalkanique*, vol. 2 (1937), pp. 77–105.

Theorem 11.14 Let **P** be the transition matrix for a regular Markov chain with fixed vector **w**. Then for any initial probability vector $\mathbf{u}, \mathbf{uP}^n \to \mathbf{w}$ as $n \to \infty$.

Proof. Let X_0, X_1, \ldots be a Markov chain with transition matrix **P** started in state s_i . Let Y_0, Y_1, \ldots be a Markov chain with transition probability **P** started with initial probabilities given by **w**. The X and Y processes are run independently of each other.

We consider also a third Markov chain \mathbf{P}^* which consists of watching both the X and Y processes. The states for \mathbf{P}^* are pairs (s_i, s_j) . The transition probabilities are given by

$$\mathbf{P}^*[(i,j),(k,l)] = \mathbf{P}(i,j) \cdot \mathbf{P}(k,l)$$

Since **P** is regular there is an N such that $\mathbf{P}^{N}(i, j) > 0$ for all *i* and *j*. Thus for the \mathbf{P}^{*} chain it is also possible to go from any state (s_i, s_j) to any other state (s_k, s_l) in at most N steps. That is \mathbf{P}^{*} is also a regular Markov chain.

We know that a regular Markov chain will reach any state in a finite time. Let T be the first time the chain \mathbf{P}^* is in a state of the form (s_k, s_k) . In other words, T is the first time that the X and the Y processes are in the same state. Then we have shown that

$$P[T > n] \to 0 \text{ as } n \to \infty$$
.

If we watch the X and Y processes after the first time they are in the same state we would not predict any difference in their long range behavior. Since this will happen no matter how we started these two processes, it seems clear that the long range behaviour should not depend upon the starting state. We now show that this is true.

We first note that if $n \ge T$, then since X and Y are both in the same state at time T,

$$P(X_n = j \mid n \ge T) = P(Y_n = j \mid n \ge T) .$$

If we multiply both sides of this equation by $P(n \ge T)$, we obtain

$$P(X_n = j, \ n \ge T) = P(Y_n = j, \ n \ge T) .$$
(11.1)

We know that for all n,

$$P(Y_n = j) = w_j \; .$$

But

$$P(Y_n = j) = P(Y_n = j, n \ge T) + P(Y_n = j, n < T)$$

and the second summand on the right-hand side of this equation goes to 0 as n goes to ∞ , since P(n < T) goes to 0 as n goes to ∞ . So,

$$P(Y_n = j, n \ge T) \to w_j$$
,

as n goes to ∞ . From Equation 11.1, we see that

$$P(X_n = j, n \ge T) \to w_j$$
,

as n goes to ∞ . But by similar reasoning to that used above, the difference between this last expression and $P(X_n = j)$ goes to 0 as n goes to ∞ . Therefore,

$$P(X_n = j) \to w_j$$
,

as n goes to ∞ . This completes the proof.

In the above proof, we have said nothing about the rate at which the distributions of the X_n 's approach the fixed distribution **w**. In fact, it can be shown that¹⁸

$$\sum_{j=1}^{r} |P(X_n = j) - w_j| \le 2P(T > n) .$$

The left-hand side of this inequality can be viewed as the distance between the distribution of the Markov chain after n steps, starting in state s_i , and the limiting distribution \mathbf{w} .

Exercises

1 Define **P** and **y** by

$$\mathbf{P} = \begin{pmatrix} .5 & .5\\ .25 & .75 \end{pmatrix}, \qquad \mathbf{y} = \begin{pmatrix} 1\\ 0 \end{pmatrix} \ .$$

Compute \mathbf{Py} , $\mathbf{P}^2\mathbf{y}$, and $\mathbf{P}^4\mathbf{y}$ and show that the results are approaching a constant vector. What is this vector?

- **2** Let **P** be a regular $r \times r$ transition matrix and **y** any *r*-component column vector. Show that the value of the limiting constant vector for $\mathbf{P}^n \mathbf{y}$ is \mathbf{wy} .
- **3** Let

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0\\ .25 & 0 & .75\\ 0 & 0 & 1 \end{pmatrix}$$

be a transition matrix of a Markov chain. Find two fixed vectors of \mathbf{P} that are linearly independent. Does this show that the Markov chain is not regular?

- 4 Describe the set of all fixed column vectors for the chain given in Exercise 3.
- 5 The theorem that $\mathbf{P}^n \to \mathbf{W}$ was proved only for the case that \mathbf{P} has no zero entries. Fill in the details of the following extension to the case that \mathbf{P} is regular. Since \mathbf{P} is regular, for some N, \mathbf{P}^N has no zeros. Thus, the proof given shows that $M_{nN} m_{nN}$ approaches 0 as n tends to infinity. However, the difference $M_n m_n$ can never increase. (Why?) Hence, if we know that the differences obtained by looking at every Nth time tend to 0, then the entire sequence must also tend to 0.
- 6 Let **P** be a regular transition matrix and let **w** be the unique non-zero fixed vector of **P**. Show that no entry of **w** is 0.

¹⁸T. Lindvall, Lectures on the Coupling Method (New York: Wiley 1992).

- 7 Here is a trick to try on your friends. Shuffle a deck of cards and deal them out one at a time. Count the face cards each as ten. Ask your friend to look at one of the first ten cards; if this card is a six, she is to look at the card that turns up six cards later; if this card is a three, she is to look at the card that turns up three cards later, and so forth. Eventually she will reach a point where she is to look at a card that turns up x cards later but there are not x cards left. You then tell her the last card that she looked at even though you did not know her starting point. You tell her you do this by watching her, and she cannot disguise the times that she looks at the cards. In fact you just do the same procedure and, even though you do not start at the same point as she does, you will most likely end at the same point. Why?
- 8 Write a program to play the game in Exercise 7.

11.5 Mean First Passage Time for Ergodic Chains

In this section we consider two closely related descriptive quantities of interest for ergodic chains: the mean time to return to a state and the mean time to go from one state to another state.

Let **P** be the transition matrix of an ergodic chain with states s_1, s_2, \ldots, s_r . Let $\mathbf{w} = (w_1, w_2, \ldots, w_r)$ be the unique probability vector such that $\mathbf{wP} = \mathbf{w}$. Then, by the Law of Large Numbers for Markov chains, in the long run the process will spend a fraction w_j of the time in state s_j . Thus, if we start in any state, the chain will eventually reach state s_j ; in fact, it will be in state s_j infinitely often.

Another way to see this is the following: Form a new Markov chain by making s_j an absorbing state, that is, define $p_{jj} = 1$. If we start at any state other than s_j , this new process will behave exactly like the original chain up to the first time that state s_j is reached. Since the original chain was an ergodic chain, it was possible to reach s_j from any other state. Thus the new chain is an absorbing chain with a single absorbing state s_j that will eventually be reached. So if we start the original chain at a state s_i with $i \neq j$, we will eventually reach the state s_j .

Let **N** be the fundamental matrix for the new chain. The entries of **N** give the expected number of times in each state before absorption. In terms of the original chain, these quantities give the expected number of times in each of the states before reaching state s_j for the first time. The *i*th component of the vector **Nc** gives the expected number of steps before absorption in the new chain, starting in state s_i . In terms of the old chain, this is the expected number of steps required to reach state s_j for the first time starting at state s_i .

Mean First Passage Time

Definition 11.7 If an ergodic Markov chain is started in state s_i , the expected number of steps to reach state s_j for the first time is called the *mean first passage time* from s_i to s_j . It is denoted by m_{ij} . By convention $m_{ii} = 0$.



Figure 11.5: The maze problem.

Example 11.24 Let us return to the maze example (Example 11.22). We shall make this ergodic chain into an absorbing chain by making state 5 an absorbing state. For example, we might assume that food is placed in the center of the maze and once the rat finds the food, he stays to enjoy it (see Figure 11.5).

The new transition matrix in canonical form is

		1	2	3	4	6	7	8	9	5	
	1	(0	1/2	0	0	1/2	0	0	0	0	
	2	1/3	0	1/3	0	0	0	0	0	1/3	
	3	0	1/2	0	1/2	0	0	0	0	0	
	4	0	0	1/3	0	0	1/3	0	1/3	1/3	
Р	= 6	1/3	0	0	0	0	0	0	0	1/3	
	7	0	0	0	0	1/2	0	1/2	0	0	
	8	0	0	0	0	0	1/3	0	1/3	1/3	
	9	0	0	0	1/2	0	0	1/2	0	0	
	5	0	0	0	0	0	0	0	0	1 /	

If we compute the fundamental matrix \mathbf{N} , we obtain

	$/^{14}$	9	4	3	9	4	3	$2 \downarrow$
	6	14	6	4	4	2	2	2
	4	9	14	9	3	2	3	4
N 1	2	4	6	14	2	2	4	6
$\mathbf{N} = \frac{1}{8}$	6	4	2	2	14	6	4	2
	4	3	2	3	9	14	9	4
	2	2	2	4	4	6	14	6
	$\backslash 2$	3	4	9	3	4	9	$_{14}/$

.

The expected time to absorption for different starting states is given by the vec-

tor Nc, where

$$\mathbf{Nc} = \begin{pmatrix} 6\\5\\6\\5\\5\\6\\5\\6 \end{pmatrix}$$

We see that, starting from compartment 1, it will take on the average six steps to reach food. It is clear from symmetry that we should get the same answer for starting at state 3, 7, or 9. It is also clear that it should take one more step, starting at one of these states, than it would starting at 2, 4, 6, or 8. Some of the results obtained from **N** are not so obvious. For instance, we note that the expected number of times in the starting state is 14/8 regardless of the state in which we start.

Mean Recurrence Time

A quantity that is closely related to the mean first passage time is the *mean recurrence time*, defined as follows. Assume that we start in state s_i ; consider the length of time before we return to s_i for the first time. It is clear that we must return, since we either stay at s_i the first step or go to some other state s_j , and from any other state s_j , we will eventually reach s_i because the chain is ergodic.

Definition 11.8 If an ergodic Markov chain is started in state s_i , the expected number of steps to return to s_i for the first time is the *mean recurrence time* for s_i . It is denoted by r_i .

We need to develop some basic properties of the mean first passage time. Consider the mean first passage time from s_i to s_j ; assume that $i \neq j$. This may be computed as follows: take the expected number of steps required given the outcome of the first step, multiply by the probability that this outcome occurs, and add. If the first step is to s_j , the expected number of steps required is 1; if it is to some other state s_k , the expected number of steps required is m_{kj} plus 1 for the step already taken. Thus,

$$m_{ij} = p_{ij} + \sum_{k \neq j} p_{ik}(m_{kj} + 1) ,$$

or, since $\sum_{k} p_{ik} = 1$,

$$m_{ij} = 1 + \sum_{k \neq j} p_{ik} m_{jk}$$
 (11.2)

Similarly, starting in s_i , it must take at least one step to return. Considering all possible first steps gives us

$$r_i = \sum_k p_{ik}(m_{ki} + 1) \tag{11.3}$$

$$= 1 + \sum_{k} p_{ik} m_{ki} . (11.4)$$

Mean First Passage Matrix and Mean Recurrence Matrix

Let us now define two matrices \mathbf{M} and \mathbf{D} . The *ij*th entry m_{ij} of \mathbf{M} is the mean first passage time to go from s_i to s_j if $i \neq j$; the diagonal entries are 0. The matrix \mathbf{M} is called the *mean first passage matrix*. The matrix \mathbf{D} is the matrix with all entries 0 except the diagonal entries $d_{ii} = r_i$. The matrix \mathbf{D} is called the *mean recurrence matrix*. Let \mathbf{C} be an $r \times r$ matrix with all entries 1. Using Equation 11.2 for the case $i \neq j$ and Equation 11.4 for the case i = j, we obtain the matrix equation

$$\mathbf{M} = \mathbf{P}\mathbf{M} + \mathbf{C} - \mathbf{D} , \qquad (11.5)$$

or

$$(\mathbf{I} - \mathbf{P})\mathbf{M} = \mathbf{C} - \mathbf{D} . \tag{11.6}$$

Equation 11.6 with $m_{ii} = 0$ implies Equations 11.2 and 11.4. We are now in a position to prove our first basic theorem.

Theorem 11.15 For an ergodic Markov chain, the mean recurrence time for state s_i is $r_i = 1/w_i$, where w_i is the *i*th component of the fixed probability vector for the transition matrix.

Proof. Multiplying both sides of Equation 11.6 by \mathbf{w} and using the fact that

$$\mathbf{w}(\mathbf{I} - \mathbf{P}) = \mathbf{0}$$

gives

$$wC - wD = 0$$
.

Here **wC** is a row vector with all entries 1 and **wD** is a row vector with *i*th entry $w_i r_i$. Thus

$$(1, 1, \dots, 1) = (w_1 r_1, w_2 r_2, \dots, w_n r_n)$$

and

 $r_i = 1/w_i \; ,$

as was to be proved.

Corollary 11.1 For an ergodic Markov chain, the components of the fixed probability vector **w** are strictly positive.

Proof. We know that the values of r_i are finite and so $w_i = 1/r_i$ cannot be 0. \Box

Example 11.25 In Example 11.22 we found the fixed probability vector for the maze example to be

$$\mathbf{w} = \begin{pmatrix} \frac{1}{12} & \frac{1}{8} & \frac{1}{12} & \frac{1}{8} & \frac{1}{6} & \frac{1}{8} & \frac{1}{12} & \frac{1}{8} & \frac{1}{12} \end{pmatrix}$$
.

Hence, the mean recurrence times are given by the reciprocals of these probabilities. That is,

$$\mathbf{r} = (12 \ 8 \ 12 \ 8 \ 6 \ 8 \ 12 \ 8 \ 12)$$
.

Returning to the Land of Oz, we found that the weather in the Land of Oz could be represented by a Markov chain with states rain, nice, and snow. In Section 11.3 we found that the limiting vector was $\mathbf{w} = (2/5, 1/5, 2/5)$. From this we see that the mean number of days between rainy days is 5/2, between nice days is 5, and between snowy days is 5/2.

Fundamental Matrix

We shall now develop a fundamental matrix for ergodic chains that will play a role similar to that of the fundamental matrix $\mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1}$ for absorbing chains. As was the case with absorbing chains, the fundamental matrix can be used to find a number of interesting quantities involving ergodic chains. Using this matrix, we will give a method for calculating the mean first passage times for ergodic chains that is easier to use than the method given above. In addition, we will state (but not prove) the Central Limit Theorem for Markov Chains, the statement of which uses the fundamental matrix.

We begin by considering the case that \mathbf{P} is the transition matrix of a regular Markov chain. Since there are no absorbing states, we might be tempted to try $\mathbf{Z} = (\mathbf{I} - \mathbf{P})^{-1}$ for a fundamental matrix. But $\mathbf{I} - \mathbf{P}$ does not have an inverse. To see this, recall that a matrix \mathbf{R} has an inverse if and only if $\mathbf{Rx} = \mathbf{0}$ implies $\mathbf{x} = \mathbf{0}$. But since $\mathbf{Pc} = \mathbf{c}$ we have $(\mathbf{I} - \mathbf{P})\mathbf{c} = \mathbf{0}$, and so $\mathbf{I} - \mathbf{P}$ does not have an inverse.

We recall that if we have an absorbing Markov chain, and \mathbf{Q} is the restriction of the transition matrix to the set of transient states, then the fundamental matrix \mathbf{N} could be written as

$$\mathbf{N} = \mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \cdots$$

The reason that this power series converges is that $\mathbf{Q}^n \to 0$, so this series acts like a convergent geometric series.

This idea might prompt one to try to find a similar series for regular chains. Since we know that $\mathbf{P}^n \to \mathbf{W}$, we might consider the series

$$\mathbf{I} + (\mathbf{P} - \mathbf{W}) + (\mathbf{P}^2 - \mathbf{W}) + \cdots$$
 (11.7)

We now use special properties of **P** and **W** to rewrite this series. The special properties are: 1) $\mathbf{PW} = \mathbf{W}$, and 2) $\mathbf{W}^k = \mathbf{W}$ for all positive integers k. These

facts are easy to verify, and are left as an exercise (see Exercise 22). Using these facts, we see that

$$(\mathbf{P} - \mathbf{W})^n = \sum_{i=0}^n (-1)^i \binom{n}{i} \mathbf{P}^{n-i} \mathbf{W}^i$$
$$= \mathbf{P}^n + \sum_{i=1}^n (-1)^i \binom{n}{i} \mathbf{W}^i$$
$$= \mathbf{P}^n + \sum_{i=1}^n (-1)^i \binom{n}{i} \mathbf{W}$$
$$= \mathbf{P}^n + \left(\sum_{i=1}^n (-1)^i \binom{n}{i}\right) \mathbf{W}$$

If we expand the expression $(1-1)^n$, using the Binomial Theorem, we obtain the expression in parenthesis above, except that we have an extra term (which equals 1). Since $(1-1)^n = 0$, we see that the above expression equals -1. So we have

$$(\mathbf{P}-\mathbf{W})^n=\mathbf{P}^n-\mathbf{W}\;,$$

for all $n \ge 1$.

We can now rewrite the series in 11.7 as

$$\mathbf{I} + (\mathbf{P} - \mathbf{W}) + (\mathbf{P} - \mathbf{W})^2 + \cdots$$

Since the *n*th term in this series is equal to $\mathbf{P}^n - \mathbf{W}$, the *n*th term goes to 0 as *n* goes to infinity. This is sufficient to show that this series converges, and sums to the inverse of the matrix $\mathbf{I} - \mathbf{P} + \mathbf{W}$. We call this inverse the *fundamental matrix* associated with the chain, and we denote it by \mathbf{Z} .

In the case that the chain is ergodic, but not regular, it is not true that $\mathbf{P}^n \to \mathbf{W}$ as $n \to \infty$. Nevertheless, the matrix $\mathbf{I} - \mathbf{P} + \mathbf{W}$ still has an inverse, as we will now show.

Proposition 11.1 Let \mathbf{P} be the transition matrix of an ergodic chain, and let \mathbf{W} be the matrix all of whose rows are the fixed probability row vector for \mathbf{P} . Then the matrix

$$I - P + W$$

has an inverse.

Proof. Let \mathbf{x} be a column vector such that

$$(\mathbf{I} - \mathbf{P} + \mathbf{W})\mathbf{x} = \mathbf{0} \ .$$

To prove the proposition, it is sufficient to show that \mathbf{x} must be the zero vector. Multiplying this equation by \mathbf{w} and using the fact that $\mathbf{w}(\mathbf{I}-\mathbf{P}) = \mathbf{0}$ and $\mathbf{w}\mathbf{W} = \mathbf{w}$, we have

$$\mathbf{w}(\mathbf{I} - \mathbf{P} + \mathbf{W})\mathbf{x} = \mathbf{w}\mathbf{x} = \mathbf{0} \; .$$

Therefore,

$$(\mathbf{I} - \mathbf{P})\mathbf{x} = \mathbf{0} \; .$$

But this means that $\mathbf{x} = \mathbf{P}\mathbf{x}$ is a fixed column vector for \mathbf{P} . By Theorem 11.10, this can only happen if \mathbf{x} is a constant vector. Since $\mathbf{w}\mathbf{x} = 0$, and \mathbf{w} has strictly positive entries, we see that $\mathbf{x} = \mathbf{0}$. This completes the proof.

As in the regular case, we will call the inverse of the matrix $\mathbf{I} - \mathbf{P} + \mathbf{W}$ the *fundamental matrix* for the ergodic chain with transition matrix \mathbf{P} , and we will use \mathbf{Z} to denote this fundamental matrix.

Example 11.26 Let \mathbf{P} be the transition matrix for the weather in the Land of Oz. Then

$$\mathbf{I} - \mathbf{P} + \mathbf{W} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} + \begin{pmatrix} 2/5 & 1/5 & 2/5 \\ 2/5 & 1/5 & 2/5 \\ 2/5 & 1/5 & 2/5 \end{pmatrix}$$
$$= \begin{pmatrix} 9/10 & -1/20 & 3/20 \\ -1/10 & 6/5 & -1/10 \\ 3/20 & -1/20 & 9/10 \end{pmatrix} ,$$

so

$$\mathbf{Z} = (\mathbf{I} - \mathbf{P} + \mathbf{W})^{-1} = \begin{pmatrix} 86/75 & 1/25 & -14/75 \\ 2/25 & 21/25 & 2/25 \\ -14/75 & 1/25 & 86/75 \end{pmatrix} .$$

Using the Fundamental Matrix to Calculate the Mean First Passage Matrix

We shall show how one can obtain the mean first passage matrix \mathbf{M} from the fundamental matrix \mathbf{Z} for an ergodic Markov chain. Before stating the theorem which gives the first passage times, we need a few facts about \mathbf{Z} .

Lemma 11.2 Let $\mathbf{Z} = (\mathbf{I} - \mathbf{P} + \mathbf{W})^{-1}$, and let \mathbf{c} be a column vector of all 1's. Then

$$\mathbf{Z}\mathbf{c} = \mathbf{c}$$
,
 $\mathbf{w}\mathbf{Z} = \mathbf{w}$.

and

$$\mathbf{Z}(\mathbf{I} - \mathbf{P}) = \mathbf{I} - \mathbf{W} \; .$$

Proof. Since $\mathbf{Pc} = \mathbf{c}$ and $\mathbf{Wc} = \mathbf{c}$,

$$\mathbf{c} = (\mathbf{I} - \mathbf{P} + \mathbf{W})\mathbf{c}$$
 .

If we multiply both sides of this equation on the left by \mathbf{Z} , we obtain

$$\mathbf{Z}\mathbf{c}=\mathbf{c}$$
 .

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Similarly, since $\mathbf{wP} = \mathbf{w}$ and $\mathbf{wW} = \mathbf{w}$,

$$\mathbf{w} = \mathbf{w}(\mathbf{I} - \mathbf{P} + \mathbf{W}) \; .$$

If we multiply both sides of this equation on the right by \mathbf{Z} , we obtain

$$\mathbf{w}\mathbf{Z} = \mathbf{w}$$
.

Finally, we have

$$\begin{aligned} (\mathbf{I} - \mathbf{P} + \mathbf{W}) (\mathbf{I} - \mathbf{W}) &= \mathbf{I} - \mathbf{W} - \mathbf{P} + \mathbf{W} + \mathbf{W} - \mathbf{W} \\ &= \mathbf{I} - \mathbf{P} \; . \end{aligned}$$

Multiplying on the left by \mathbf{Z} , we obtain

$$\mathbf{I} - \mathbf{W} = \mathbf{Z}(\mathbf{I} - \mathbf{P}) \; .$$

This completes the proof.

The following theorem shows how one can obtain the mean first passage times from the fundamental matrix.

Theorem 11.16 The mean first passage matrix \mathbf{M} for an ergodic chain is determined from the fundamental matrix \mathbf{Z} and the fixed row probability vector \mathbf{w} by

$$m_{ij} = \frac{z_{jj} - z_{ij}}{w_j} \; .$$

Proof. We showed in Equation 11.6 that

$$(\mathbf{I} - \mathbf{P})\mathbf{M} = \mathbf{C} - \mathbf{D} \ .$$

Thus,

$$\mathbf{Z}(\mathbf{I} - \mathbf{P})\mathbf{M} = \mathbf{Z}\mathbf{C} - \mathbf{Z}\mathbf{D} \ ,$$

and from Lemma 11.2,

$$\mathbf{Z}(\mathbf{I}-\mathbf{P})\mathbf{M}=\mathbf{C}-\mathbf{Z}\mathbf{D}~.$$

Again using Lemma 11.2, we have

$$\mathbf{M} - \mathbf{W}\mathbf{M} = \mathbf{C} - \mathbf{Z}\mathbf{D}$$

or

$$\mathbf{M} = \mathbf{C} - \mathbf{Z}\mathbf{D} + \mathbf{W}\mathbf{M}$$

From this equation, we see that

$$m_{ij} = 1 - z_{ij}r_j + (\mathbf{wM})_j$$
 (11.8)

But $m_{jj} = 0$, and so

$$0 = 1 - z_{jj}r_j + (\mathbf{wM})_j ,$$

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or

$$(\mathbf{wM})_j = z_{jj}r_j - 1$$
 . (11.9)

From Equations 11.8 and 11.9, we have

Since
$$r_j = 1/w_j$$
,

$$m_{ij} = \frac{z_{jj} - z_{ij}}{w_j} \ .$$

Example 11.27 (Example 11.26 continued) In the Land of Oz example, we find that (25/75 - 1/25 - 1/4/75)

 $m_{ij} = (z_{jj} - z_{ij}) \cdot r_j \; .$

$$\mathbf{Z} = (\mathbf{I} - \mathbf{P} + \mathbf{W})^{-1} = \begin{pmatrix} 86/75 & 1/25 & -14/75 \\ 2/25 & 21/25 & 2/25 \\ -14/75 & 1/25 & 86/75 \end{pmatrix} .$$

We have also seen that $\mathbf{w} = (2/5, 1/5, 2/5)$. So, for example,

$$m_{12} = \frac{z_{22} - z_{12}}{w_2}$$
$$= \frac{21/25 - 1/25}{1/5}$$
$$= 4 ,$$

by Theorem 11.16. Carrying out the calculations for the other entries of \mathbf{M} , we obtain

$$\mathbf{M} = \begin{pmatrix} 0 & 4 & 10/3 \\ 8/3 & 0 & 8/3 \\ 10/3 & 4 & 0 \end{pmatrix} \ .$$

Computation

The program **ErgodicChain** calculates the fundamental matrix, the fixed vector, the mean recurrence matrix \mathbf{D} , and the mean first passage matrix \mathbf{M} . We have run the program for the Ehrenfest urn model (Example 11.8). We obtain:

		0	1	2	3	4	
	0	(.0000	1.0000	.0000	.0000	.0000 \	
	1	.2500	.0000	.7500	.0000	.0000	
$\mathbf{P} =$	2	.0000	.5000	.0000	.5000	.0000	;
	3	.0000	.0000	.7500	.0000	.2500	
	4	0000.	.0000	.0000	1.0000	.0000/	
					2		
		0	1	2	3	4	
w	=	(.0625	.2500	.3750	.2500	.0625);	

$$\mathbf{M} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ \mathbf{r} = & (16.0000 & 4.0000 & 2.6667 & 4.0000 & 16.0000); \\ 0 & 1 & 2 & 3 & 4 \\ 0 & (10000 & 1.0000 & 2.6667 & 6.3333 & 21.3333) \\ 15.0000 & .0000 & 1.6667 & 5.3333 & 20.3333) \\ 18.6667 & 3.6667 & .0000 & 3.6667 & 18.6667 \\ 20.3333 & 5.3333 & 1.6667 & .0000 & 15.0000 \\ 21.3333 & 6.3333 & 2.6667 & 1.0000 & .0000 \end{pmatrix}.$$

From the mean first passage matrix, we see that the mean time to go from 0 balls in urn 1 to 2 balls in urn 1 is 2.6667 steps while the mean time to go from 2 balls in urn 1 to 0 balls in urn 1 is 18.6667. This reflects the fact that the model exhibits a central tendency. Of course, the physicist is interested in the case of a large number of molecules, or balls, and so we should consider this example for n so large that we cannot compute it even with a computer.

Ehrenfest Model

Example 11.28 (Example 11.23 continued) Let us consider the Ehrenfest model (see Example 11.8) for gas diffusion for the general case of 2n balls. Every second, one of the 2n balls is chosen at random and moved from the urn it was in to the other urn. If there are *i* balls in the first urn, then with probability i/2n we take one of them out and put it in the second urn, and with probability (2n - i)/2n we take a ball from the second urn and put it in the first urn. At each second we let the number *i* of balls in the first urn be the state of the system. Then from state *i* we can pass only to state i - 1 and i + 1, and the transition probabilities are given by

$$p_{ij} = \begin{cases} \frac{i}{2n} , & \text{if } j = i - 1, \\ 1 - \frac{i}{2n} , & \text{if } j = i + 1, \\ 0 , & \text{otherwise.} \end{cases}$$

This defines the transition matrix of an ergodic, non-regular Markov chain (see Exercise 15). Here the physicist is interested in long-term predictions about the state occupied. In Example 11.23, we gave an intuitive reason for expecting that the fixed vector \mathbf{w} is the binomial distribution with parameters 2n and 1/2. It is easy to check that this is correct. So,

$$w_i = \frac{\binom{2n}{i}}{2^{2n}}$$

Thus the mean recurrence time for state i is

$$r_i = \frac{2^{2n}}{\binom{2n}{i}} \ .$$



Figure 11.6: Ehrenfest simulation.

Consider in particular the central term i = n. We have seen that this term is approximately $1/\sqrt{\pi n}$. Thus we may approximate r_n by $\sqrt{\pi n}$.

This model was used to explain the concept of reversibility in physical systems. Assume that we let our system run until it is in equilibrium. At this point, a movie is made, showing the system's progress. The movie is then shown to you, and you are asked to tell if the movie was shown in the forward or the reverse direction. It would seem that there should always be a tendency to move toward an equal proportion of balls so that the correct order of time should be the one with the most transitions from i to i - 1 if i > n and i to i + 1 if i < n.

In Figure 11.6 we show the results of simulating the Ehrenfest urn model for the case of n = 50 and 1000 time units, using the program **EhrenfestUrn**. The top graph shows these results graphed in the order in which they occurred and the bottom graph shows the same results but with time reversed. There is no apparent difference.

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We note that if we had not started in equilibrium, the two graphs would typically look quite different. $\hfill \Box$

Reversibility

If the Ehrenfest model is started in equilibrium, then the process has no apparent time direction. The reason for this is that this process has a property called *reversibility*. Define X_n to be the number of balls in the left urn at step n. We can calculate, for a general ergodic chain, the reverse transition probability:

$$P(X_{n-1} = j | X_n = i) = \frac{P(X_{n-1} = j, X_n = i)}{P(X_n = i)}$$
$$= \frac{P(X_{n-1} = j)P(X_n = i | X_{n-1} = j)}{P(X_n = i)}$$
$$= \frac{P(X_{n-1} = j)p_{ji}}{P(X_n = i)}.$$

In general, this will depend upon n, since $P(X_n = j)$ and also $P(X_{n-1} = j)$ change with n. However, if we start with the vector \mathbf{w} or wait until equilibrium is reached, this will not be the case. Then we can define

$$p_{ij}^* = \frac{w_j p_{ji}}{w_i}$$

as a transition matrix for the process watched with time reversed.

Let us calculate a typical transition probability for the reverse chain $\mathbf{P}^* = \{p_{ij}^*\}$ in the Ehrenfest model. For example,

$$p_{i,i-1}^* = \frac{w_{i-1}p_{i-1,i}}{w_i} = \frac{\binom{2n}{i-1}}{2^{2n}} \times \frac{2n-i+1}{2n} \times \frac{2^{2n}}{\binom{2n}{i}}$$
$$= \frac{(2n)!}{(i-1)!(2n-i+1)!} \times \frac{(2n-i+1)i!(2n-i)!}{2n(2n)!}$$
$$= \frac{i}{2n} = p_{i,i-1} .$$

Similar calculations for the other transition probabilities show that $\mathbf{P}^* = \mathbf{P}$. When this occurs the process is called *reversible*. Clearly, an ergodic chain is reversible if, and only if, for every pair of states s_i and s_j , $w_i p_{ij} = w_j p_{ji}$. In particular, for the Ehrenfest model this means that $w_i p_{i,i-1} = w_{i-1} p_{i-1,i}$. Thus, in equilibrium, the pairs (i, i-1) and (i-1, i) should occur with the same frequency. While many of the Markov chains that occur in applications are reversible, this is a very strong condition. In Exercise 12 you are asked to find an example of a Markov chain which is not reversible.

The Central Limit Theorem for Markov Chains

Suppose that we have an ergodic Markov chain with states s_1, s_2, \ldots, s_k . It is natural to consider the distribution of the random variables $S_i^{(n)}$, which denotes

the number of times that the chain is in state s_j in the first n steps. The *j*th component w_j of the fixed probability row vector \mathbf{w} is the proportion of times that the chain is in state s_j in the long run. Hence, it is reasonable to conjecture that the expected value of the random variable $S_j^{(n)}$, as $n \to \infty$, is asymptotic to nw_j , and it is easy to show that this is the case (see Exercise 23).

It is also natural to ask whether there is a limiting distribution of the random variables $S_j^{(n)}$. The answer is yes, and in fact, this limiting distribution is the normal distribution. As in the case of independent trials, one must normalize these random variables. Thus, we must subtract from $S_j^{(n)}$ its expected value, and then divide by its standard deviation. In both cases, we will use the asymptotic values of these quantities, rather than the values themselves. Thus, in the first case, we will use the value nw_j . It is not so clear what we should use in the second case. It turns out that the quantity

$$\sigma_j^2 = 2w_j z_{jj} - w_j - w_j^2 \tag{11.10}$$

represents the asymptotic variance. Armed with these ideas, we can state the following theorem.

Theorem 11.17 (Central Limit Theorem for Markov Chains) For an ergodic chain, for any real numbers r < s, we have

$$P\left(r < \frac{S_j^{(n)} - nw_j}{\sqrt{n\sigma_j^2}} < s\right) \to \frac{1}{\sqrt{2\pi}} \int_r^s e^{-x^2/2} \, dx \; ,$$

as $n \to \infty$, for any choice of starting state, where σ_j^2 is the quantity defined in Equation 11.10.

Historical Remarks

Markov chains were introduced by Andree Andreevich Markov (1856–1922) and were named in his honor. He was a talented undergraduate who received a gold medal for his undergraduate thesis at St. Petersburg University. Besides being an active research mathematician and teacher, he was also active in politics and patricipated in the liberal movement in Russia at the beginning of the twentieth century. In 1913, when the government celebrated the 300th anniversary of the House of Romanov family, Markov organized a counter-celebration of the 200th anniversary of Bernoulli's discovery of the Law of Large Numbers.

Markov was led to develop Markov chains as a natural extension of sequences of independent random variables. In his first paper, in 1906, he proved that for a Markov chain with positive transition probabilities and numerical states the average of the outcomes converges to the expected value of the limiting distribution (the fixed vector). In a later paper he proved the central limit theorem for such chains. Writing about Markov, A. P. Youschkevitch remarks:

Markov arrived at his chains starting from the internal needs of probability theory, and he never wrote about their applications to physical

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science. For him the only real examples of the chains were literary texts, where the two states denoted the vowels and consonants.¹⁹

In a paper written in 1913,²⁰ Markov chose a sequence of 20,000 letters from Pushkin's *Eugene Onegin* to see if this sequence can be approximately considered a simple chain. He obtained the Markov chain with transition matrix

	vowel	$\operatorname{consonant}$		
vowel	(.128	.872		
$\operatorname{consonant}$.663	.337)		

The fixed vector for this chain is (.432, .568), indicating that we should expect about 43.2 percent vowels and 56.8 percent consonants in the novel, which was borne out by the actual count.

Claude Shannon considered an interesting extension of this idea in his book *The Mathematical Theory of Communication*,²¹ in which he developed the information-theoretic concept of entropy. Shannon considers a series of Markov chain approximations to English prose. He does this first by chains in which the states are letters and then by chains in which the states are words. For example, for the case of words he presents first a simulation where the words are chosen independently but with appropriate frequencies.

REPRESENTING AND SPEEDILY IS AN GOOD APT OR COME CAN DIFFERENT NATURAL HERE HE THE A IN CAME THE TO OF TO EXPERT GRAY COME TO FURNISHES THE LINE MES-SAGE HAD BE THESE.

He then notes the increased resemblence to ordinary English text when the words are chosen as a Markov chain, in which case he obtains

THE HEAD AND IN FRONTAL ATTACK ON AN ENGLISH WRI-TER THAT THE CHARACTER OF THIS POINT IS THEREFORE ANOTHER METHOD FOR THE LETTERS THAT THE TIME OF WHO EVER TOLD THE PROBLEM FOR AN UNEXPECTED.

A simulation like the last one is carried out by opening a book and choosing the first word, say it is *the*. Then the book is read until the word *the* appears again and the word after this is chosen as the second word, which turned out to be *head*. The book is then read until the word *head* appears again and the next word, *and*, is chosen, and so on.

Other early examples of the use of Markov chains occurred in Galton's study of the problem of survival of family names in 1889 and in the Markov chain introduced

 ¹⁹See Dictionary of Scientific Biography, ed. C. C. Gillespie (New York: Scribner's Sons, 1970),
 pp. 124–130.
 ²⁰A. A. Markov, "An Example of Statistical Analysis of the Text of Eugene Onegin Illustrat-

²⁰A. A. Markov, "An Example of Statistical Analysis of the Text of Eugene Onegin Illustrating the Association of Trials into a Chain," *Bulletin de l'Acadamie Imperiale des Sciences de St. Petersburg*, ser. 6, vol. 7 (1913), pp. 153–162.

 $^{^{21}}$ C. E. Shannon and W. Weaver, *The Mathematical Theory of Communication* (Urbana: Univ. of Illinois Press, 1964).

by P. and T. Ehrenfest in 1907 for diffusion. Poincaré in 1912 dicussed card shuffling in terms of an ergodic Markov chain defined on a permutation group. Brownian motion, a continuous time version of random walk, was introducted in 1900–1901 by L. Bachelier in his study of the stock market, and in 1905–1907 in the works of A. Einstein and M. Smoluchowsky in their study of physical processes.

One of the first systematic studies of finite Markov chains was carried out by M. Frechet.²² The treatment of Markov chains in terms of the two fundamental matrices that we have used was developed by Kemeny and Snell²³ to avoid the use of eigenvalues that one of these authors found too complex. The fundamental matrix N occurred also in the work of J. L. Doob and others in studying the connection between Markov processes and classical potential theory. The fundamental matrix Z for ergodic chains appeared first in the work of Frechet, who used it to find the limiting variance for the central limit theorem for Markov chains.

Exercises

1 Consider the Markov chain with transition matrix

$$\mathbf{P} = \begin{pmatrix} 1/2 & 1/2 \\ 1/4 & 3/4 \end{pmatrix}$$

Find the fundamental matrix \mathbf{Z} for this chain. Compute the mean first passage matrix using \mathbf{Z} .

- 2 A study of the strengths of Ivy League football teams shows that if a school has a strong team one year it is equally likely to have a strong team or average team next year; if it has an average team, half the time it is average next year, and if it changes it is just as likely to become strong as weak; if it is weak it has 2/3 probability of remaining so and 1/3 of becoming average.
 - (a) A school has a strong team. On the average, how long will it be before it has another strong team?
 - (b) A school has a weak team; how long (on the average) must the alumni wait for a strong team?
- **3** Consider Example 11.4 with a = .5 and b = .75. Assume that the President says that he or she will run. Find the expected length of time before the first time the answer is passed on incorrectly.
- **4** Find the mean recurrence time for each state of Example 11.4 for a = .5 and b = .75. Do the same for general a and b.
- **5** A die is rolled repeatedly. Show by the results of this section that the mean time between occurrences of a given number is 6.

²²M. Frechet, "Théorie des événements en chaine dans le cas d'un nombre fini d'états possible," in *Recherches théoriques Modernes sur le calcul des probabilités*, vol. 2 (Paris, 1938).

²³J. G. Kemeny and J. L. Snell, *Finite Markov Chains*.



Figure 11.7: Maze for Exercise 7.

- 6 For the Land of Oz example (Example 11.1), make rain into an absorbing state and find the fundamental matrix **N**. Interpret the results obtained from this chain in terms of the original chain.
- 7 A rat runs through the maze shown in Figure 11.7. At each step it leaves the room it is in by choosing at random one of the doors out of the room.
 - (a) Give the transition matrix **P** for this Markov chain.
 - (b) Show that it is an ergodic chain but not a regular chain.
 - (c) Find the fixed vector.
 - (d) Find the expected number of steps before reaching Room 5 for the first time, starting in Room 1.
- 8 Modify the program **ErgodicChain** so that you can compute the basic quantities for the queueing example of Exercise 11.3.20. Interpret the mean recurrence time for state 0.
- **9** Consider a random walk on a circle of circumference n. The walker takes one unit step clockwise with probability p and one unit counterclockwise with probability q = 1 p. Modify the program **ErgodicChain** to allow you to input n and p and compute the basic quantities for this chain.
 - (a) For which values of n is this chain regular? ergodic?
 - (b) What is the limiting vector **w**?
 - (c) Find the mean first passage matrix for n = 5 and p = .5. Verify that $m_{ij} = d(n-d)$, where d is the clockwise distance from i to j.
- 10 Two players match pennies and have between them a total of 5 pennies. If at any time one player has all of the pennies, to keep the game going, he gives one back to the other player and the game will continue. Show that this game can be formulated as an ergodic chain. Study this chain using the program ErgodicChain.

- 11 Calculate the reverse transition matrix for the Land of Oz example (Example 11.1). Is this chain reversible?
- 12 Give an example of a three-state ergodic Markov chain that is not reversible.
- 13 Let **P** be the transition matrix of an ergodic Markov chain and \mathbf{P}^* the reverse transition matrix. Show that they have the same fixed probability vector **w**.
- 14 If **P** is a reversible Markov chain, is it necessarily true that the mean time to go from state i to state j is equal to the mean time to go from state j to state i? *Hint*: Try the Land of Oz example (Example 11.1).
- 15 Show that any ergodic Markov chain with a symmetric transition matrix (i.e., $p_{ij} = p_{ji}$) is reversible.
- 16 (Crowell²⁴) Let \mathbf{P} be the transition matrix of an ergodic Markov chain. Show that

$$(\mathbf{I} + \mathbf{P} + \dots + \mathbf{P}^{n-1})(\mathbf{I} - \mathbf{P} + \mathbf{W}) = \mathbf{I} - \mathbf{P}^n + n\mathbf{W}$$
,

and from this show that

$$\frac{\mathbf{I} + \mathbf{P} + \dots + \mathbf{P}^{n-1}}{n} \to \mathbf{W} ,$$

as $n \to \infty$.

- 17 An ergodic Markov chain is started in equilibrium (i.e., with initial probability vector **w**). The mean time until the next occurrence of state s_i is $\bar{m}_i = \sum_k w_k m_{ki} + w_i r_i$. Show that $\bar{m}_i = z_{ii}/w_i$, by using the facts that $\mathbf{wZ} = \mathbf{w}$ and $m_{ki} = (z_{ii} z_{ki})/w_i$.
- 18 A perpetual craps game goes on at Charley's. Jones comes into Charley's on an evening when there have already been 100 plays. He plans to play until the next time that snake eyes (a pair of ones) are rolled. Jones wonders how many times he will play. On the one hand he realizes that the average time between snake eyes is 36 so he should play about 18 times as he is equally likely to have come in on either side of the halfway point between occurrences of snake eyes. On the other hand, the dice have no memory, and so it would seem that he would have to play for 36 more times no matter what the previous outcomes have been. Which, if either, of Jones's arguments do you believe? Using the result of Exercise 17, calculate the expected to reach snake eyes, in equilibrium, and see if this resolves the apparent paradox. If you are still in doubt, simulate the experiment to decide which argument is correct. Can you give an intuitive argument which explains this result?
- **19** Show that, for an ergodic Markov chain (see Theorem 11.16),

$$\sum_{j} m_{ij} w_j = \sum_{j} z_{jj} - 1 = K \; .$$

 $^{^{24}\}mathrm{Private}$ communication.

- 5	20
B	C
- 30	15
A	GO

Figure 11.8: Simplified Monopoly.

The second expression above shows that the number K is independent of i. The number K is called *Kemeny's constant*. A prize was offered to the first person to give an intuitively plausible reason for the above sum to be independent of i. (See also Exercise 24.)

20 Consider a game played as follows: You are given a regular Markov chain with transition matrix **P**, fixed probability vector **w**, and a payoff function **f** which assigns to each state s_i an amount f_i which may be positive or negative. Assume that $\mathbf{wf} = 0$. You watch this Markov chain as it evolves, and every time you are in state s_i you receive an amount f_i . Show that your expected winning after n steps can be represented by a column vector $\mathbf{g}^{(n)}$, with

$$\mathbf{g}^{(n)} = (\mathbf{I} + \mathbf{P} + \mathbf{P}^2 + \dots + \mathbf{P}^n)\mathbf{f}.$$

Show that as $n \to \infty$, $\mathbf{g}^{(n)} \to \mathbf{g}$ with $\mathbf{g} = \mathbf{Z}\mathbf{f}$.

- 21 A highly simplified game of "Monopoly" is played on a board with four squares as shown in Figure 11.8. You start at GO. You roll a die and move clockwise around the board a number of squares equal to the number that turns up on the die. You collect or pay an amount indicated on the square on which you land. You then roll the die again and move around the board in the same manner from your last position. Using the result of Exercise 20, estimate the amount you should expect to win in the long run playing this version of Monopoly.
- 22 Show that if **P** is the transition matrix of a regular Markov chain, and **W** is the matrix each of whose rows is the fixed probability vector corresponding to **P**, then $\mathbf{PW} = \mathbf{W}$, and $\mathbf{W}^k = \mathbf{W}$ for all positive integers k.
- **23** Assume that an ergodic Markov chain has states s_1, s_2, \ldots, s_k . Let $S_j^{(n)}$ denote the number of times that the chain is in state s_j in the first *n* steps. Let **w** denote the fixed probability row vector for this chain. Show that, regardless of the starting state, the expected value of $S_j^{(n)}$, divided by *n*, tends to w_j as $n \to \infty$. *Hint*: If the chain starts in state s_i , then the expected value of $S_j^{(n)}$ is given by the expression

$$\sum_{h=0}^{n} p_{ij}^{(h)}$$

24 Peter Doyle²⁵ has suggested the following interpretation for Kemeny's constant (see Exercise 19). We are given an ergodic chain and do not know the starting state. However, we would like to start watching it at a time when it can be considered to be in equilibrium (i.e., as if we had started with the fixed vector \mathbf{w} or as if we had waited a long time). However, we don't know the starting state and we don't want to wait a long time. Peter says to choose a state according to the fixed vector \mathbf{w} . That is, choose state j with probability w_j using a spinner, for example. Then wait until the time T that this state occurs for the first time. We consider T as our starting time and observe the chain from this time on. Of course the probability that we start in state jis w_j , so we are starting in equilibrium. Kemeny's constant is the expected value of T, and it is independent of the way in which the chain was started. Should Peter have been given the prize?

 $^{^{25}\}mathrm{Private}$ communication.