

# Markov Chains: Examples with Theory

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## Preface

Welcome to *Markov Chains: Examples with Theory*. Before launching into the content, take some time to learn my purpose in writing it, the audience I intended, and why a math book contains so many computer programs.

One day when I mentioned that I was working on this book, my wife asked me “Who are you writing this for?”. Without thinking too hard, I quickly answered “Myself”. My interests over the last 10 years have ranged over the mathematics underneath bioinformatics and political redistricting. In mathematically understanding both of these widely separated topics, large Markov chains are an essential tool. Although I had the usual basic knowledge about small Markov chains, I did not think I really understood large Markov chains. So I began studying large chains and eventually realized that my notes had a logical order as a book.

A quote from the well-known mathematician and author Paul Halmos captures the spirit of this book:

A good stack of examples, as large as possible, is indispensable for a thorough understanding of any concept, and when I want to learn something new, I make it my first job to build one.

The stack of examples here are explicit Markov chains, mostly from familiar contexts, progressing from small state spaces to large state spaces. Many books on Markov chains present examples with small state spaces for the admirable reason that readers can grasp the ideas and compute the required quantities by hand. With modern computing power and with improved algorithms it is now possible to directly compute required quantities in chains with hundreds, thousands, or even millions of states. These examples are scattered throughout the literature and on the internet. Part of the goal is to present this “stack of examples” with unified notation and common vocabulary to make understanding the subject as a whole easier. The ultimate goal is to bring the reader (and myself) to the point of being able to read modern and advanced books on Markov chains and research papers on Markov chains. The examples help evaluate and confirm the advanced topics.

Each chapter has the same components. Each chapter starts with an introductory paragraph or two followed by a difficulty rating. In teaching and reading, I have found it useful to give an idea of what is ahead. So I assign one of four ratings to each chapter:

- Everyone: contains no mathematics, suitable for general reading.
- Student: contains scenes of mild algebra or calculus that may require guidance.
- Mathematically Mature: contains mathematics beyond calculus with proofs. This generally means mathematics up to the fourth-year level covered in an American university.
- Mathematicians Only: prolonged scenes of intense rigor. This generally means mathematics covered in graduate level courses.

Immediately after the chapter introduction is a Starter Question. This is for the reader to warm up and think critically about the topic. The main part of each chapter follows in several sections, written in a mildly formal, but not terse, Definition-Theorem-Proof-Remark style. This main part concludes with my answer to the Starter Question. Since the Starter Questions are open-ended, the answers are not definitive, and the reader may have valid answers which are shorter, longer or even different. The Chapter Ending Answers usually involve results from the main body of the Chapter, so the reader is not necessarily going to be able to answer. Remember, the Starter Questions are just intended to get the reader thinking critically about the chapter topic. Each chapter finishes with a summary of the definitions, vocabulary, and the notations. Illustrating a main idea from the chapter is an Algorithm and one or more programs, currently in the R programming language. The Algorithm gives the idea for the program in pseudocode. Finally there are a few exercises for the reader, some of which fill in details from the chapter.

Although the book leads to large Markov chains, two small examples appear wherever they are useful. The first is the almost trivial “weather in Oz” example which appears in many treatments of Markov chains. This small but useful example introduces concepts understandable almost at a glance. The second example appearing throughout is the Ehrenfest urn model. This canonical example is non-trivial but still can be understood with hand calculations.

Some features of the text are a little unusual. The first is that numerous or detailed theorem hypotheses and longer proofs are broken into short numbered steps. The goal is to make the points short, easily-digested, identifiable and modular. Numbered items help the reader follow along step by step. If the reader gets lost, it is easier to refer to a step by number rather than “the next to last sentence in the first paragraph.” Enumerating the steps also makes the proofs more detailed with fewer gaps. The second is that except for this preface there are no first person pronouns. I try to present the subject just as it is without injecting personalities. I hope the reader finds this factual and helpful, not impersonal. The third feature is an emphasis on calculating variance and covariance of the random variables when possible, not just the expected value. Finally, important theorems have names but most of the names are my creation, not standard names in the literature. It is easier to remember and refer to the “Fundamental Theorem of Markov Chains” than Theorem 1.11. I don’t expect these theorem names to become common, theorems

are named here to mark them as important and worthy of use by name elsewhere in the text.

This text is more explicit about mathematical details, generally not skipping over steps. This makes the text longer than it would be in a printed edition. The omission of details may be an advantage with a paper book, saving cost and weight. High-quality electronic presentations in book format eliminate the need for space-saving omissions.

To a reasonable extent, each chapter follows the pedagogical Rule of Three (or four). That is, the discussion should be symbolic, visual or graphic, and numeric (and explained verbally). The symbolic is the traditional mathematical style, the visual or graphical for Markov chains generally schematic rather than directly representational and the numeric is achieved through short computer programs.

It is now fashionable to make videos explaining all sorts of topics. I believe the video format is not suitable for deep mathematical ideas and examples. An extended long format text with a table of contents, an index, numbered theorems, illustrations, tables, and lengthy explanations allow the reader the chance to stop, think, calculate, and re-read if necessary. I believe a text such as this is the best form for the topic of Markov chains with examples and theory.

## Intended Audience and Background

This book is primarily for beginning graduate students in mathematics and mathematicians who want to learn about Markov chains in detail. Learners in physical sciences, computer science, economics, and engineering will also benefit from the book with its examples of Markov chains.

This book is for students after courses on calculus-based probability theory and linear algebra. To understand the explanations, theorems, proofs and to complete the exercises:

- (1) The reader should understand probability theory including distributions, random variables, and elementary random processes.
- (2) The reader should understand linear algebra and matrix theory, including eigenvalues and eigenvectors.
- (3) The reader should understand real analysis, including  $\epsilon - \delta$  style proofs of convergence. Understanding asymptotics is necessary in Part 2, including  $O(n)$  and  $o(n)$  style notation. Measure-theoretic probability appears in only a few places.
- (4) The reader should be familiar with common statistical concepts of parameter point evaluations and confidence intervals and hypothesis testing.

## Notational Conventions

- (1) The sequence of random variables for a Markov chain is  $X_n$ , the state space for the random variables is  $\mathcal{X}$  and the values in the state space are  $x_i, x_j$  and so on.

- (2) The variables  $i$ ,  $j$  and  $\ell$  are generic variables representing states if the state space context is clear or unnecessary.
- (3)  $\Omega$  is the underlying sample space, and in particular for applications in statistical mechanics and related areas  $\Omega$  is the total configuration space.
- (4) The variables  $n$  and  $m$  are generic variables for discrete values, usually times or indices.
- (5) If  $\mathcal{X}$  is finite, its cardinality is  $k = \text{card}(\mathcal{X})$ .
- (6) The variable  $\nu$  is exclusively used as a dummy variable of summation whenever the index of summation has no immediate interpretation. Sometimes  $\mu$  is also used as a dummy variable of summation.
- (7)  $P$  is the transition probability matrix for a Markov chain.  $Q$  is a related, derived, or auxiliary transition probability matrix.
- (8) The stationary distribution for a Markov chain is  $\boldsymbol{\pi}$ . Math boldface for this distribution or vector distinguishes it from the mathematical constant and also from the symbol of a permutation from the symmetric group.
- (9)  $\tau$  with or without a subscript is a random time or a stopping time (except when discussing the symmetric group where it denotes an arbitrary permutation and one chapter where  $\tau$  is the standard notation for a normal population precision, the reciprocal of the variance.)

## Program Scripts

An important feature of this book is the simulation scripts that accompany most sections. The simulation scripts illustrate the concepts and theorems of the section with numerical and graphical evidence. The scripts are part of the “Rule of 3” teaching philosophy of presenting mathematical ideas symbolically, numerically and graphically.

The programs are springboards for further experimentation, not finished apps for everyday use. The scripts are minimal in size, in scope of implementation and with minimal output. The scripts are not complete, stand-alone, polished applications, rather they are proof-of-concept starting points. The reader should run the scripts to illustrate the ideas and provide numerical examples of the results in the section. The scripts provide a seed for new scripts to increase the size and scope of the simulations. Increasing the size can often demonstrate convergence or increase confidence in the results of the section. Increasing the size can also demonstrate that although convergence is mathematically guaranteed, sometimes the rate of convergence is slow. The reader is also encouraged to change the output, to provide more information, to add different graphical representations, and to investigate rates of convergence.

The scripts are not specifically designed to be efficient, either in program language implementation or in mathematical algorithm. Efficiency is not ignored, but it is not the primary consideration in the construction of the scripts. Similarity of the program algorithm to the mathematical idea takes precedence over efficiency. One noteworthy aspect of both the similarity and efficiency is that all the languages use vectorization along with other notational simplifications such as

recycling. Vectorized scripts look more like the mathematical expressions found in the text, making the code easier to understand. Vectorized code often runs much faster.

The scripts minimize using additional language packages and add-ons, instead relying on the base language as much as possible. Some packages, particularly for Markov chain simulations and for linear algebra, are too useful to ignore and so the scripts use these mature packages judiciously. Avoiding simplifying packages sometimes has the consequence of making the scripts longer, or more complicated, or less efficient. On the other hand, for the reader interested in immediately applying the scripts, it eliminates the need for searching for and installing packages, some of which might be specialized, obscure, even outdated. Also, since plotting varies so much by language, graphics format, operating system, even available hardware or resources, most scripts avoid plotting or make only the simplest plots. The reader is encouraged to try additional language packages to make the scripts easier to read, or more efficient. The reader is also encouraged to make plots of the calculated quantities, using available plotting software or language packages. Since many of the scripts rely on independent samples, those scripts can be made to run faster by using parallelization of the sampling. The reader is encouraged to experiment with parallelization in the code.

The scripts are not intended to be a tutorial on how to do mathematical programming in any of the languages. A description of the algorithm used in the scripts is in each section. The description is usually in full sentences rather than the more formal symbolic representation found in computer science pseudo-code. Given the description and some basic awareness of programming ideas, the scripts provide multiple examples for study. The scripts provide a starting point for investigating, testing and comparing language features from the documentation or from other sources. The scripts use good programming style whenever possible, but clarity, simplicity and similarity to the mathematics are primary considerations.

*Disclaimer.* The final preparation of this text happened at the same time that generative large language models (sometimes called AI) became widely available. Although these models can summarize large volumes of information, they do so with the possibility of errors, even “hallucinations”. Not a single word of this text was written with the help of a generative large language model. Any mistakes are entirely my own.





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*Part 1*

## **Basic Examples and Theory**



# Markov Chains

This chapter is a survey of basic concepts and facts about discrete time Markov processes and Markov chains. Detailed treatments are in [Dur09, Fel73, GS97, KT75, KST74, KS60, LPW09, Ros06, Sti05], among other standard references.

Mathematically Mature: contains mathematics beyond calculus with proofs.

## 1.1. Chapter Starter Question

Consider the magical Land of Oz where the weather follows a pattern. If it is raining today, then there is a 50% chance of raining again tomorrow, and a 25% chance of either having a nice day or a snowy day tomorrow. Similarly if it is snowing today, there is a 50% chance of having snow tomorrow, and a 25% chance of either having a nice day, or a rainy day tomorrow. Also the land of Oz never has two nice days in a row, with equal chance of rain or snow the day after a nice day. What is the chance it is nice in two days given it is rainy today?

## 1.2. Introduction

Begin by understanding where Markov chains fit in the larger landscape of probability theory.

**Definition 1.1.** A **stochastic process** is a random function on a domain. The domain can be discrete or continuous. The domain is often interpreted as time. Stochastic processes are in contrast to deterministic processes. An outcome of the stochastic process at some time must be specified in terms of the probability of it happening.  $\diamond$

**Example 1.2.** Consider the following simple example:

$$f(t) = 2t$$

$$g(t) = \begin{cases} 2t & \text{with probability 0.98} \\ 3t & \text{with probability 0.02.} \end{cases}$$

For  $f(2)$  the outcome will always be 4, it is deterministic. However for  $g(2)$  the most likely outcome is 4 but this will fail to be true for about 2% of the trials.  $\nabla$

**Definition 1.3.** The outcome of a **discrete time discrete state space stochastic process** is one of several discrete states at a sequence of discrete times. The set of states is  $\mathcal{X} = \{x_1, x_2, \dots, x_i, \dots\}$ . Sometimes the discrete state space  $\mathcal{X}$  is infinite, but often the state space is finite. The sequence of discrete times is  $\{t_0, t_1, \dots, t_n, \dots\}$ . Often the precise times are not needed, so the sequence of events is indicated with  $1, 2, \dots, n, \dots$ . At time  $n$ , guided by some information, the process acts in a probabilistic manner and outputs some  $x_i$ . Thus along a specific sample, as time progresses an observed sequence of states from the set  $\mathcal{X}$  is a **sample path**.  $\diamond$

**Definition 1.4.** A **discrete time Markov process**  $X_n$  is a stochastic process having a fixed probability that it will be in state  $x_j$  at time  $n+1$  when the process is in state  $x_i$  at time  $n$ , with no dependence on the prior history. Symbolically,

$$\mathbb{P}[X_{t_{n+1}} \mid X_{t_n} = x_n, X_{t_{n-1}} = x_{n-1}, \dots, X_{t_1} = x_1, X_{t_0} = x_0] = \mathbb{P}[X_{t_{n+1}} \mid X_{t_n} = x_n]$$

Denote the probability of making the transition from state  $x_i$  to  $x_j$  at time  $n$  as:

$$P_{ij}(n) = \mathbb{P}[X_{n+1} = x_j \mid X_n = x_i].$$

Note that already the exact times have been dropped and replaced with their sequence position.  $\diamond$

**Example 1.5.** As a contrast, consider a discrete time stochastic process modeling the daily closing price of a company's stock. At time  $n$ , there is a wealth of available information influencing the current price: the past prices of the stock, the current market conditions, even the weather forecast for the next few days. Without simplifying assumptions, stock prices would not be a Markov process.

Instead, simplify by modeling the daily closing price of a stock as a *discrete time Markov process*, at time  $n+1$  the *only* information that would affect the process would be the observed stock price at time  $n$ .  $\nabla$

**Definition 1.6.** If the probability of a state transition in a Markov process does not depend on  $n$ , then it is a **time-homogeneous Markov chain**. This means  $P_{ij}(n) = P_{ij}(m)$  for all  $n, m$ . That is, the transition probabilities from  $x_i$  to  $x_j$  are time invariant with fixed  $P_{ij}$ , called the transition probabilities from  $x_i$  to  $x_j$ . If the state space is finite, say  $\text{card}(\mathcal{X}) = k$ , then the  $P_{ij}$  are the entries of an  $k \times k$  matrix  $P$  called the **transition probability matrix**.  $\diamond$

**Definition 1.7.** A **stochastic matrix** is a square matrix with non-negative entries for which all the rows sum to 1.

### 1.3. Example of a Markov Chain

The following is a classic example from [KST74], repeated in [GS97] and many other locations. The example shows the concepts in context as well as introducing some other ideas.

**Example 1.8.** Consider the magical Land of Oz where the weather follows a pattern. If it is raining today, then there is a 50% chance of raining again tomorrow, and a 25% chance of either having a nice day or a snowy day tomorrow. Similarly if it is snowing, there is a 50% chance of again having snow, and a 25% chance of either having a nice day, or a rainy day. The land of Oz never has two nice days in a row, and Oz equally has rain and snow the day after a nice day.

First label the states conveniently as  $R, N, S$ , instead of  $x_1, x_2, x_3$ . With the information above, define  $P_{RR} = 1/2$ ,  $P_{RN} = 1/4$  and so on. Writing out every possible transition gives  $3^2$  distinct possibilities. With  $k$  states, the process has  $k^2$  transitions with the probability  $P_{ij}$  of going from  $x_i$  to  $x_j$ .

Use matrices to represent the transition probabilities for the Markov chain. In the example, the transition matrix is (the row and column labels of  $R, N$  and  $S$  are for convenience only and are not usually included in the display of the matrix)

$$P = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} \end{matrix}.$$

Note that all the rows sum to 1, thus this is a *stochastic matrix*.

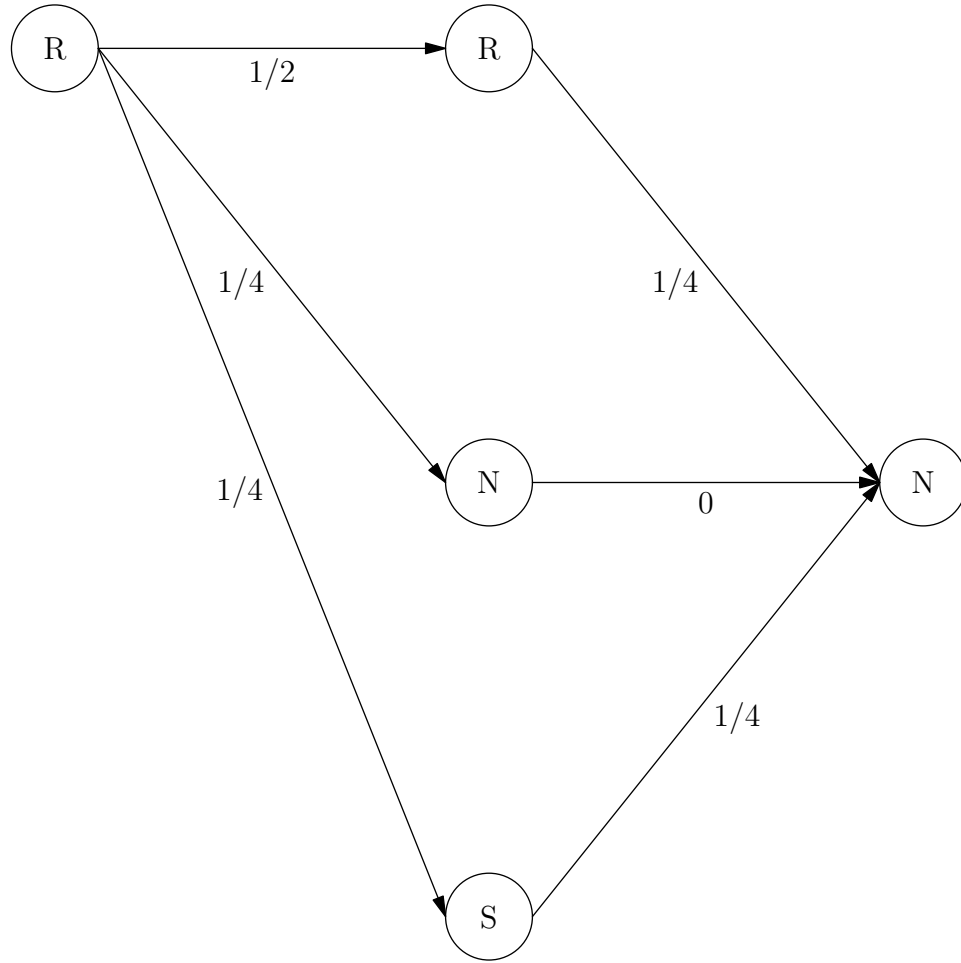
How to calculate the chance it is nice in two days given it is rainy today? Use the Law of Total Probability, considering every possible weather combination with their respective conditional probabilities. See Figure 1.1 for a diagram of the combination process. Mixing the  $R = x_1$ ,  $N = x_2$ ,  $S = x_3$  notation, this example has

$$\mathbb{P}[X_{n+2} = N | X_n = R] = \sum_{\nu=1}^3 P_{1\nu} P_{\nu 2}.$$

For two days, this is not too tedious, but what about the probability it will be nice a week from today given it is rainy today?

Now matrix notation is convenient. Notice that the probability above of going from  $R$  to  $N$  two days hence is the  $(1, 2)$  entry in the matrix product of  $P$  with itself. More generally, the transition probability through  $n$  steps is the matrix  $P^n$ , and this is known as (the finite Markov chain version of) the *Chapman-Kolmogorov Theorem*. Thus consider the following matrices from the example:

$$P^2 = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 7/16 & 3/16 & 6/16 \\ 6/16 & 4/16 & 6/16 \\ 6/16 & 3/16 & 7/16 \end{pmatrix} \end{matrix}$$



**Figure 1.1.** A schematic diagram of the calculation of the two-step transition probability.

and

$$P^7 = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 0.400024 & 0.200012 & 0.399963 \\ 0.400024 & 0.199951 & 0.400024 \\ 0.399963 & 0.200012 & 0.400024 \end{pmatrix} \end{matrix}.$$

If it is raining today, then the chance it is nice in 2 and 7 days is  $3/16$  and  $0.200012$  respectively.  $\nabla$

#### 1.4. Formal Definitions

Let the state space be a finite set  $\mathcal{X} = \{x_1, x_2, \dots, x_k\}$ .

**Definition 1.9.** A **Markov chain** is a discrete time discrete state space stochastic process defined by its transition probability matrix  $P$  with entries

$$P_{ij}(n) = \mathbb{P}[X_{n+1} = x_j \mid X_n = x_i].$$

The entries must satisfy  $P_{ij} \geq 0$  and  $\sum_{\nu=1}^k P_{i\nu} = 1$  for each  $i = 1, \dots, k$ , so that each row is a probability distribution on  $\mathcal{X}$ .  $\diamond$

This means that the Markov chain is a random walk among the states with dependence only on the current state. If  $x_i$  is the current state, choose  $x_j$  with probability  $P_{ij}$ ; from  $x_j$  choose  $x_l$  with probability  $P_{jl}$ , and so on. The sequence of outcomes  $X_0 = x_i, X_1 = x_j, X_2 = x_l \dots$  is a **sample path** of the Markov chain.

In terms of conditional probabilities,

$$\begin{aligned} \mathbb{P}[X_1 = x_j \mid X_0 = x_i] &= P_{ij} \\ \mathbb{P}[X_2 = x_l, X_1 = x_j \mid X_0 = x_i] &= P_{ij}P_{jl}. \end{aligned}$$

Then combining over all the intermediate possibilities

$$\mathbb{P}[X_2 = x_l \mid X_0 = x_i] = \sum_{j=1}^k P_{ij}P_{jl}$$

which is matrix multiplication. This is the *Chapman-Kolmogorov equation* for finite Markov chains. Extending this observation by induction

$$\mathbb{P}[X_n = j \mid X_0 = i] = (P^n)_{ij}$$

the  $i, j$  entry of the  $n$ th power of  $P$ .

**Definition 1.10.** A Markov chain has a **stationary distribution** if there is a vector  $\boldsymbol{\pi}$  satisfying

$$\sum_{i=1}^k \boldsymbol{\pi}_i P_{ij} = \boldsymbol{\pi}_j$$

with  $\boldsymbol{\pi}_i > 0$ , and  $\sum_{i=1}^k \boldsymbol{\pi}_i = 1$ .

Thus  $\boldsymbol{\pi}$  is a left eigenvector of  $P$  with eigenvalue 1. The Perron Theorem guarantees that such a left eigenvector exists for transition probability matrices. Alternative terminology is that the Markov chain is **stable on the distribution**  $\boldsymbol{\pi}$  and that  $\boldsymbol{\pi}$  is the **stable distribution** for the Markov chain. The probabilistic interpretation of the left eigenvector equation is “pick  $x_i$  from  $\mathcal{X}$  with probability  $\boldsymbol{\pi}_i$  and take a step with probability  $P_{ij}$ , the probability of being at  $x_j$  is  $\boldsymbol{\pi}_j$ ”. Thus  $\boldsymbol{\pi}$  is stationary for the evolution of the Markov chain.

The Fundamental Theorem of Markov Chains guarantees that a stable distribution always exists under reasonable conditions. The precise definitions of the conditions on a Markov chain for the following Fundamental Theorem to hold are in the next chapter “Classes of States and Stationary Distributions”. The proof of the Fundamental Theorem is also in the next chapter “Classes of States and Stationary Distributions”.



**Theorem 1.11** (Fundamental Theorem of Markov Chains). *For an irreducible, positive recurrent and aperiodic Markov chain,  $\lim_{n \rightarrow \infty} (P^n)_{ij}$  exists and is independent of  $i$ . Furthermore, letting*

$$\pi_j = \lim_{n \rightarrow \infty} (P^n)_{ij}$$

*then  $\pi_j$  is the unique non-negative solution of*

$$\begin{aligned} \sum_i \pi_i P_{ij} &= \pi_j, \\ \sum_i \pi_i &= 1. \end{aligned}$$

An irreducible, positive recurrent and aperiodic Markov chain with transition matrix  $P$  has the following property: As  $n \rightarrow \infty$ , the matrix  $P^n$  approaches a limiting matrix  $P^\infty$ , where  $P^\infty$  consists of  $n$  copies of the same row vector. This matrix has different names in different texts, two common names are the “limit matrix”, or the matrix of “limiting probabilities.”

The probabilistic content of the Fundamental Theorem is that from any starting state  $x_i$ , for large  $n$  the  $n$ th step of a sample path of the Markov chain has a probability close to  $\pi_j$  of being at  $x_j$ . Later chapters address the question of what “probability close to  $\pi_j$ ” means and how large  $n$  must be for this probability relationship to hold.

**Example 1.12.** For the weather in Oz example, consider  $P^7$  further:

$$P^7 = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 0.400024 & 0.200012 & 0.399963 \\ 0.400024 & 0.199951 & 0.400024 \\ 0.399963 & 0.200012 & 0.400024 \end{pmatrix} \end{matrix}.$$

Note that the chance of being in any of the three states after seven days is almost independent of the initial state. This means the weather in seven days is almost completely independent of what it is today. Considering  $P^n$  for larger values of  $n$ , the row vectors approach  $\pi = (2/5, 1/5, 2/5)$ .  $\nabla$

**Example 1.13.** Convergence to a stationary distribution works for the weather example, but it will not work for every matrix. Consider:

$$Q = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

This matrix describes a two-state system switching states at each time step. Thus  $Q^2 = I$ ,  $Q^3 = Q$ ,  $Q^4 = I$  and so on. This particular matrix does not have the aperiodic property so it does not satisfy the requirements of the Fundamental Theorem.  $\nabla$

## 1.5. Absorbing States

Up to this point the main example has been an irreducible, positive recurrent, and aperiodic Markov chain. Now consider the following transition probability matrix:

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

Note that if the process starts in state  $x_1$  or  $x_5$ , it can't leave these states. Similarly, if the process starts in any other state and “arrives” in states  $x_1$  or  $x_5$  at time  $N$ , then it stays in those states for all steps  $n \geq N$ . Call these **absorbing states**, that is, states which once entered are never left. All other states are **transient states**.

The transition probability matrix  $P$  represents the symmetric random walk on  $x_1, x_2, x_3, x_4, x_5$  that stops at  $x_1$  or  $x_5$ . Markov chains with absorbing states are *not* irreducible. Therefore the Fundamental Theorem does not apply for a limit matrix. Instead introduce the **transition probability matrix canonical form**. Given a Markov chain defined by transition matrix  $P$  with  $a$  absorbing states and  $t$  transient states where  $a + t = k$ , then after reordering the states the matrix has the canonical form

$$P = \begin{pmatrix} I & 0 \\ A & T \end{pmatrix}$$

where  $I$  is the  $a \times a$  identity matrix, and  $0$  is the  $a \times t$  matrix of zeros. The random walk matrix from above has the canonical form after reordering to  $x_1, x_5, x_2, x_3, x_4$ . :

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

The canonical form of the transition probability matrix ordering the absorbing states first is common in theoretical treatments and in software packages implementing Markov chains. However in some contexts, especially games and sports, it is more convenient to order the transient starting states first and put the end absorbing states of winning or losing as the last of the states. The Markov chain then “flows” from the start state of the game to some end state. Then the canonical form becomes

$$P = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix}.$$

The matrix  $N = (I - T)^{-1}$  (or  $N = (I - Q)^{-1}$ ) is called the **fundamental matrix**. The chapter on “Waiting Time to Absorption” proves that entry  $N_{ij}$  of the fundamental matrix is the expected number of times the chain will be at state

$x_j$  before absorption, given it started in state  $x_i$ . So in the random walk example:

$$N = (I - T)^{-1} = \begin{pmatrix} 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 3/2 \end{pmatrix}.$$

Letting  $\mathbf{1}$  be the  $1 \times t$  vector of all ones,  $\mathbf{1}N$  is the vector with the expected number of steps for the transient state to be absorbed in one of the absorbing states, in this case  $(3, 4, 3)$ . Define  $B = NA$ , so  $B_{ij}$  is the probability that starting in the  $i$ th transient state, the process ends up in the  $j$ th absorbing state. In the example:

$$B = (I - T)^{-1}A = \begin{pmatrix} 3/4 & 1/4 \\ 1/2 & 1/2 \\ 1/4 & 3/4 \end{pmatrix}.$$

The canonical form gives information about  $P^n$  for large values of  $n$ . As  $n \rightarrow \infty$ ,  $P^n$  approaches the matrix

$$P^\infty = \begin{pmatrix} I & 0 \\ B & 0 \end{pmatrix}.$$

## 1.6. Chapter Ending Answer

Use the Law of Total Probability to calculate this probability. This considers every possible weather combination with their respective conditional probabilities.

$$\mathbb{P}[X_2 = N \mid X_0 = R] = \frac{1}{2} \cdot \frac{1}{4} + \frac{1}{4} \cdot 0 + \frac{1}{4} \cdot \frac{1}{4} = \frac{3}{16}.$$

## 1.7. Chapter Summary

### Key Concepts.

- (1) A **stochastic process** is a random function on a domain. The domain can be discrete or continuous. The domain is often interpreted as time. Stochastic processes are in contrast to deterministic processes. A specific outcome of the process at some time must be specified in terms of the probability of it happening.
- (2) A discrete time discrete state space stochastic process is a **Markov chain** if  $\mathbb{P}[X_{n+1} \mid X_n, X_{n-1}, \dots, X_1] = \mathbb{P}[X_{n+1} \mid X_n]$ . That is, the conditional probability depends only on the immediately preceding state, not the history.
- (3) Denote the probability of making the transition from state  $x_i$  to  $x_j$  at time  $n$  as:

$$P_{ij}(n) = \mathbb{P}[X_{n+1} = x_j \mid X_n = x_i].$$

If the probability of a state transition in a Markov process does not depend on  $n$ , then it is a **time-homogeneous Markov chain**. If the state space is finite, say  $\text{card}(\mathcal{X}) = k$ , then the  $p_{ij}$  are the entries of an  $k \times k$  matrix  $P$  called the **transition probability matrix**.

- (4) The transition probability for multiple time steps is the matrix  $P^n$ , and this is known as (the finite Markov chain version of) the *Chapman-Kolmogorov Theorem*.

- (5) The Fundamental Theorem of Markov Chains says: Let  $\mathcal{X}$  be a finite state space and let  $P_{ij}$  define a Markov chain on  $x_i$ . If the Markov chain is irreducible, positive recurrent and aperiodic, then  $P$  has a unique stationary distribution  $\pi$ , and as  $n \rightarrow \infty$ ,  $(P^n)_{ij} \rightarrow \pi_j$  for each  $i, j$ .
- (6) **Absorbing states** are states that once entered are never left.
- (7) Absorption probabilities can be found by putting the matrix in **canonical form**, then finding the **fundamental matrix**, and then multiplying blocks from the canonical matrix.

### Vocabulary.

- (1) A **stochastic process** is a random function on a domain.
- (2) The outcome of a **discrete time discrete state space process** is one of several states at a sequence of times. Along a specific sample, as time progresses the observed sequence of states from the set  $\mathcal{X}$  is a **sample path**.
- (3) The outcome of a **discrete time discrete state space stochastic process** is one of several discrete states at a sequence of discrete times.
- (4) A **discrete time Markov process** is a stochastic process having a fixed probability that it will be in state  $x_j$  at time  $n+1$  when the process is in state  $x_i$  at time  $n$ , with no dependence on the prior history.
- (5) If the probability of a state transition in a Markov process does not depend on  $n$ , it is a **time-homogeneous Markov chain**.
- (6) If the values in each the rows of a matrix sum to 1, it is a **stochastic matrix**.
- (7) A **Markov chain** is a discrete time discrete state space stochastic process defined by its transition probability matrix  $P$  with entries

$$P_{ij}(n) = \mathbb{P}[X_{n+1} = x_j \mid X_n = x_i].$$

The entries must satisfy  $P_{ij} \geq 0$  and  $\sum_{\nu=1}^k P_{i\nu} = 1$  for each  $i = 1, \dots, k$ , so that each row is a probability distribution on  $X$ .

- (8) The sequence of states  $X_0 = x_i, X_1 = x_j, X_2 = x_l \dots$  is a **sample path** of the Markov chain.
- (9) A chain is **ergodic**, also called **irreducible**, if it has only one communicating class.
- (10) An irreducible, positive recurrent, and aperiodic Markov chain has a **stationary distribution**  $\pi$  with  $\pi_i > 0$  satisfying

$$\sum_{i=1}^k \pi_i P_{ij} = \pi_j$$

$$\sum_{i=1}^k \pi_i = 1.$$

Thus  $\pi$  is a left eigenvector of  $P$  with eigenvalue 1. Alternative terminology is that the Markov chain is **stable on the distribution**  $\pi$  and that  $\pi$  is the **stable distribution** for the Markov chain.

- (11) States which once entered are never left are **absorbing states**.

- (12) Given a Markov chain defined by transition matrix  $P$  with  $a$  absorbing states and  $t$  non-absorbing states where  $a+t = k$ , then the matrix has the **transition probability matrix canonical form**

$$P = \begin{pmatrix} I & 0 \\ R & Q \end{pmatrix}$$

where  $I$  is the  $u \times u$  identity matrix, and  $0$  is the  $u \times v$  matrix of zeros. The matrix  $N = (I - Q)^{-1}$  is called the **fundamental matrix**.

#### Notation.

- (1)  $\mathcal{X} = \{x_1, x_2, \dots, x_i, \dots\}$  – state space of a discrete space stochastic process
- (2)  $\text{card}(\mathcal{X}) = k$  – cardinality of a finite state space
- (3)  $P$  –  $k \times k$  transition probability matrix
- (4)  $\nu$  – A dummy variable for summation
- (5)  $i, j$  – arbitrary or generic state indices
- (6)  $(P^n)_{ij}$  – the  $i, j$  entry of the  $n$ th power of  $P$ .
- (7)  $\pi$  – stationary distribution satisfying

$$\sum_{\nu=1}^k \pi_{\nu} P_{\nu j} = \pi_j$$

with  $\pi_{\nu} > 0$ , and  $\sum_{\nu=1}^k \pi_{\nu} = 1$

(8)

$$P = \begin{pmatrix} I & 0 \\ A & T \end{pmatrix}$$

– canonical form for the transition matrix  $P$  with  $a$  absorbing states and  $t$  transient states where  $a + t = k$ , where  $I$  is the  $a \times a$  identity matrix, and  $0$  is the  $a \times t$  matrix of zeros.

### 1.8. Sources

This section is adapted from: Notes prepared by LT Grant and used with permission. Pieces of this section are adapted from: *Finite Markov Chains*, Kemeny and Snell, 1960, and from *Random Walks and Electric Networks*, Doyle and Snell, 1984, as well as *A First Course in Stochastic Processes* by S. Karlin and H. Taylor, Chapter 2, 1975.

### 1.9. Links

- (1) *Introduction to Probability*, Grinstead and Snell. Chapter 11 - Markov Chains <http://tinyurl.com/qw6sa> Introduction to Probability, Chapter 11 Accessed Wed Jan 16 07:32:50 CST 2019
- (2) Markov The markovchain package Accessed Wed Jan 16 07:34:15 CST 2019
- (3) Getting Started with Markov Chains Accessed Wed Jan 16 07:32:22 CST 2019

## 1.10. Algorithms and Scripts

**Data:** State names and transition probability matrix

**Result:** Information about a simple Markov chain

- 1 *Initialization and sample paths*
- 2 Load Markov chain library
- 3 Set state names, set transition probability matrix, set start state
- 4 Set an example length and create a sample path of example length
- 5 Create a second sample path of example length
- 6 *Simulation of stationary distribution and comparison to theoretical*
- 7 Set a long path length, and a transient time
- 8 Create a long sample path
- 9 Slice the long sample path from the transient time to the end
- 10 In the slice count the appearance of each state
- 11 Store in an empirical array
- 12 Compute the theoretical stable array
- 13 **return** *Stable distribution and theoretical stable distribution*

**Algorithm 1:** Markov chain simulation.

### Scripts.

**R:** R script for markovchain.

```

1 library(markovchain)
2
3 stateNames <- c("R", "N", "S")
4 transMatrix <- matrix( c(1/2, 1/4, 1/4, 1/2, 0, 1/2,
5                          1/4, 1/4, 1/2),
6                        nrow=3, byrow=TRUE)
7
8 startState <- "N"
9
10 weather0z <- new("markovchain", transitionMatrix=
11   transMatrix,
12   states=stateNames, name="Weather_in_
13   0z")
14 print( weather0z )
15
16 print( summary(weather0z) )
17
18 pathLength <- 10
19 weatherPath <- rmarkovchain(n=pathLength,
20   object = weather0z, t0 =
21   startState)
22 cat("A sample starting from N: ", weatherPath, "\n")
23 weatherPath <- rmarkovchain(n=pathLength,
24   object = weather0z, t0 =
25   startState)

```

```

20 cat("Another sample starting from N: ", weatherPath,
    "\n")
21
22 largeN <- 1000; startStable <- 100
23 weatherPath <- rmarkovchain(n=largeN,
24                             object = weather0z, t0 =
    startState)
25 stablePattern <- weatherPath[startStable:largeN]
26 empiricalStable <- c( mean( stablePattern == "R" ),
27                      mean( stablePattern == "N" ),
28                      mean( stablePattern == "S" ))
29 theorStable <- steadyStates(weather0z)
30 cat("Empirical stable distribution: ",
    empiricalStable, "\n")
31 cat("Theoretical stable distribution: ", theorStable,
    "\n")

```

### 1.11. Problems to Work for Understanding

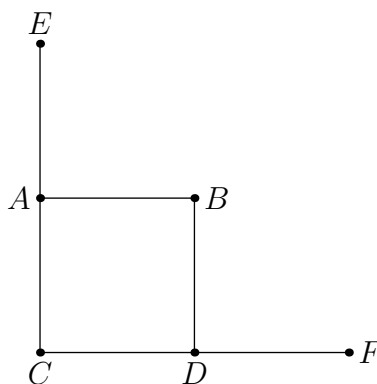
Chapter 1: Markov Chains.

1.1: Students' progress through a (two-year) Associate Degree program is not always a two year process. A student taking first year courses has a 15% chance of dropping out, a 25% chance of repeating the first year, and a 60% chance of moving on to the second year. A student taking second year material has a 10% chance of dropping out, a 20% of repeating the second year, and a 70% chance of graduating.

- How many states are in this model?
- Which states are absorbing? Which are transient?
- What is the chance a student entering the program this year will graduate "on time"? What is the chance a student will graduate in 3 years?
- What is the chance that a student will graduate eventually? What is the chance the student will drop out?
- What is the expected time until a student graduates?

1.2: Consider the grid in Figure 1.2 upon which a random walker is stuck. If she reaches states  $E$  and  $F$  she will stop, otherwise she will keep walking. At any of the other states, she is equally likely to choose any of the possible neighboring states.

- What is the transition matrix?
- What are the absorbing states? The transient states?
- What is the canonical form of this matrix? The fundamental form?
- Starting at state  $A$ , on average, how many steps will the walker take before reaching states  $E$  or  $F$ ?
- Starting at state  $A$ , what is the probability the walker will end at the state  $F$ ? Starting at  $D$  what is the probability the walker ends at state  $E$ ? Discuss these two answers.



**Figure 1.2.** Grid for the random walk.

1.3: The walker returns a year later to the same grid, only to find that there now exists a road between  $B$  and  $E$ .

- (a) Without any calculations, how would you expect this to change the absorption probabilities of state  $B$ ?
- (b) Without any calculations, would you expect the same results as you found in 2(e) above?
- (c) Find the new transition matrix.
- (d) Calculate the actual probabilities for part (a) and (b) and comment on your results.

1.4: What is the transition probability matrix for the following Markov chain?  $N$  black balls and  $N$  white balls are placed in two urns so that each contains  $N$  balls. At each step one ball is selected at random from each urn and the two balls interchange urns. The state of the system is the number of white balls in the first urn. What are the absorbing states and transient states?

1.5: What is the transition probability matrix for the following Markov chain? Consider two urns A and B with a total of  $N$  balls. An experiment is performed in which a ball is selected at random (all selections equally likely) at time  $n$ ,  $n = 1, 2, \dots$  from among the totality of  $N$  balls. Then an urn is selected at random, urn A with probability  $p$  and urn B with probability  $q = 1 - p$  and the ball previously drawn is placed in this urn. The state of the system is the number of balls in the urn A. What are the absorbing states and transient states, if any?

1.6: What is the transition probability matrix for the following Markov chain? Consider two urns A and B with a total of  $N$  balls. An experiment is performed in which an urn is selected at random in proportion to its contents (i.e. if urn A has exactly  $i$  balls, then it is selected with probability  $i/N$ ). Then a ball is selected from A with probability  $p$  and from urn B with probability  $q = 1 - p$  and placed in the previously chosen urn. The state of the system is the number of balls in the urn A. What are the absorbing states and transient states, if any?



1.7: Your baby is learning to walk. The baby begins by holding onto a couch. Whenever she is next to the couch, there is a 25% chance that she will take a step forward and a 75% percent chance that she will stay clutching the couch. If the baby is one or more steps away from the couch, there is a 25% chance that she will take a step forward, a 25% chance she will stay in place and a 50% chance she will take one step back toward the couch. In the long run, what percent of the time does the baby choose to clutch the couch?

1.8: Louie lives in a town that has a 50 percent chance of rain each morning and an independent 40 percent chance each evening. Louie walks to and from work each day, bringing an umbrella with him if it is raining and not bringing one if it isn't. On Sunday night, 2 of his 3 umbrellas were with him at home and 1 was at his office. What were the chances that he made it through the work week without getting wet?

1.9: Describe a Markov chain which has an infinite absorbing set and a Markov chain with infinitely many absorbing sets.

# Classes of States and Stationary Distributions

The states of a Markov chain partition into equivalence classes according to their type: communicating, periodic versus aperiodic, recurrent versus transient, or positive recurrent versus null recurrent. This chapter investigates the relationships among these classes. The chapter concludes with several proofs of the Fundamental Theorem of Markov Chains.

Mathematicians Only: prolonged scenes of intense rigor.

## 2.1. Chapter Starter Question

Randomly distribute three balls between two urns, labeled  $A$  and  $B$ . Each period, select an urn at random, and if it is not empty, remove a ball from that urn and put it in the other urn. How can you find the fraction of time urn  $A$  is empty? What is that fraction of time? Does this depend on how the balls are initially distributed between the two urns?

## 2.2. Classification of States

**Definition 2.1.** State  $j$  is **accessible** from state  $i$  if  $(P^n)_{ij} > 0$  for some  $n \geq 1$ . That is, state  $j$  is accessible from state  $i$  if and only if it is possible that the process will enter state  $j$  in  $n$  steps, for some  $n$ .  $\diamond$

**Definition 2.2.** Two states **communicate** if state  $j$  is accessible from state  $i$  and state  $i$  is accessible from  $j$ .  $\diamond$

**Remark 2.3.** Note that it is possible that  $j$  is accessible from  $i$  but that  $i$  and  $j$  do not communicate. An example is if  $j$  is an absorbing state accessible from  $i$ .

**Proposition 2.4.** *Communicating is an equivalence relation, so that the states of a Markov chain partition into disjoint communicating classes.*

**Proof. Reflexive:** If  $i$  communicates with itself, then  $i$  is accessible from  $i$  in  $n$  steps, and so  $i$  is accessible from itself again in  $n$  steps, so communication is reflexive.

**Symmetric:** If  $i$  and  $j$  communicate, then state  $j$  is accessible from state  $i$  in  $n_{ij}$  steps and state  $i$  is accessible from state  $j$  in  $n_{ji}$  steps. Therefore, state  $i$  is accessible from state  $j$  in  $n_{ji}$  steps and state  $j$  is accessible from state  $i$  in  $n_{ij}$  steps. That is, communication between  $i$  and  $j$  is a symmetric relation.

**Transitive:** If  $i$  communicates with  $j$  and  $j$  communicates with  $l$ , then  $(P^{n_{ij}})_{ij} > 0$  for some  $n_{ij} \geq 1$ , and likewise  $(P^{n_{jl}})_{jl} > 0$  for some  $n_{jl} \geq 1$ . Then  $(P^{n_{ij}+n_{jl}})_{il} \geq (P^{n_{ij}})_{ij}(P^{n_{jl}})_{jl} > 0$  and so it is possible that the process can enter state  $l$  from  $i$  in  $n = n_{ij} + n_{jl}$  steps, so  $l$  is accessible from  $i$ . Likewise,  $(P^{n_{lj}})_{lj} > 0$  for some  $n_{lj} \geq 1$ , and  $(P^{n_{ji}})_{ji} > 0$  for some  $n_{ji} \geq 1$ . Then  $(P^{n_{lj}})_{lj}(P^{n_{ji}})_{ji} > 0$  and so it is possible that the process can enter state  $i$  in  $n = n_{lj} + n_{ji}$  steps, so  $i$  is accessible from  $l$ . That is,  $i$  and  $l$  communicate and communication is transitive.  $\square$

**Definition 2.5.** The period of a state  $i$ , written as  $d(i)$ , is the greatest common divisor of all integers  $n \geq 1$  for which  $(P^n)_{ii} > 0$ . If  $(P^n)_{ii} = 0$  for all  $n$ , define  $d(i) = 0$ .  $\diamond$

**Proposition 2.6.** (1) If  $i$  communicates with  $j$ , then  $d(i) = d(j)$ .

(2) If state  $i$  has period  $d(i)$ , then there exists an integer  $N$  depending on  $i$  such that for all integers  $n \geq N$ ,  $(P^{nd(i)})_{ii} > 0$ . That is, return to state  $i$  can occur at all sufficiently large multiples of the period  $d(i)$ .

(3) If  $(P^m)_{ij} > 0$ , then  $(P^{m+nd(i)})_{ij} > 0$  for all sufficiently large  $n$ .

**Remark 2.7.** The proofs of the second and third parts rely on the next lemma from number theory, a generalization of a standard result about the greatest common divisor of two integers.

**Lemma 2.8.** Let  $n_1, n_2, \dots, n_s$  be positive integers with greatest common divisor  $d$ . Then there exists a positive integer  $M$  such that if  $m \geq M$  then there exist nonnegative integers  $c_1, c_2, \dots, c_s$  such that

$$md = \sum_{\nu=1}^s c_\nu n_\nu.$$

**Proof.** (1) Let

$$A = \{n : n = c_1 n_1 + \dots + c_s n_s, c_s \text{ nonnegative integers}\}$$

and

$$B = \{b_1 m_1 + \dots + b_j m_j : m_i \in A, b_i \in \mathbb{Z}, j \geq 1, i = 1, \dots, j\}.$$

(2) Let  $d'$  be the least positive integer in  $B$ , where  $d' = b_1 m'_1 + \dots + b_j m'_j$ . Since  $m'_i \in A$  for all  $i$ , each can be written as  $m'_i = c'_{1i} n_1 + \dots + c'_{si} n_s$ .

- (3) The first claim is that  $d'$  is a common divisor of all elements of  $A$ . To prove the claim, let  $a = c_1n_1 + \cdots + c_sn_s \in A$ . By the Division Algorithm let  $a = d'q + r$  with  $0 \leq r < d'$ . Then

$$\begin{aligned} r &= a - d'q \\ &= a - q(b_1m'_1 + \cdots + b_jm'_j) \\ &= (c_1n_1 + \cdots + c_sn_s) - q\left(\sum_{i=1}^j b_i \sum_{\nu=1}^s c'_{\nu i} n_\nu\right) \\ &= \left(c_1 - q \sum_{i=1}^j b_i c'_{1i}\right) n_1 + \cdots + \left(c_s - q \sum_{i=1}^j b_i c'_{si}\right) n_s. \end{aligned}$$

- (4) This means that  $r \in B$  (with  $m_i = 1 \cdot n_i \in A$  and  $b_i = c_i - q \sum_{\nu=1}^j b_\nu c'_{i\nu}$ ). Since  $0 \leq r < d'$ , and  $d'$  is the least *positive* integer in  $B$ , then  $r = 0$  and  $d'$  is a divisor of  $a$ , establishing the first claim.
- (5) For simplicity drop the prime on  $d'$  so  $d = d' = \gcd(n_1, \dots, n_s)$ . As in the previous step, rearrange the terms in the representation of  $d = b'_1m_1 + \cdots + b'_jm_j = \alpha_1n_1 + \cdots + \alpha_sn_s$  so that the terms with positive coefficients are written first. Thus  $d' = N_1 - N_2$  with  $N_1 \in A$  and  $N_2 \in A$ . Let  $M$  be the positive integer  $N_2^2/d$  (a positive integer since  $d'$  is a divisor of  $N_2 \in A$ ). Every integer  $m \geq M$  can be written as  $m = M + K = N_2^2/d + K$ , with  $K \geq 0$ . Using the Division Algorithm  $K = q'(N_2/d) + r'$  with  $0 \leq r' < N_2/d$  and the integer  $q' = \lfloor K/(N_2/d) \rfloor$ . Now

$$\begin{aligned} md &= (N_2^2/d + q'N_2/d + r')d \\ &= N_2^2 + q'N_2 + r'd \\ &= N_2^2 + q'N_2 + r'(N_1 - N_2) \\ &= N_2(N_2 + q' - r') + r'N_1. \end{aligned}$$

Recall that  $r' < N_2/d$ , so  $r' \leq N_2$ .

- (6) Since  $N_2 \in A$  and  $N_1 \in A$ , the previous step shows there exist nonnegative integers  $c_1, c_2, \dots, c_s$  such that

$$md = \sum_{\nu=1}^s c_\nu n_\nu.$$

□

**Proof of Proposition 2.6.** (1) (a) If  $i$  communicates with  $j$ , then  $(P^{n_{ij}})_{ij} > 0$  for some  $n_{ij} \geq 1$  and  $(P^{n_{ji}})_{ji} > 0$  for some  $n_{ji} \geq 1$ . Additionally since  $i$  and  $j$  communicate,  $(P^{n_{ii}})_{ii} > 0$  for some  $n_{ii}$ .

(b) Then

$$(P^{n_{ji}+n_{ii}+n_{ij}})_{jj} \geq (P^{n_{ji}})_{ji} \cdot (P^{n_{ii}})_{ii} \cdot (P^{n_{ij}})_{ij} > 0.$$

Furthermore,  $(P^{2n_{ii}})_{ii} \geq (P^{n_{ii}})_{ii} \cdot (P^{n_{ii}})_{ii} > 0$ , so

$$(P^{n_{ji}+2n_{ii}+n_{ij}})_{jj} \geq (P^{n_{ji}})_{ji} \cdot (P^{2n_{ii}})_{ii} \cdot (P^{n_{ij}})_{ij} > 0.$$

- (c) This means that  $d(j)$  divides  $n_{ji} + n_{ii} + n_{ij}$  and  $d(j)$  divides  $n_{ji} + 2n_{ii} + n_{ij}$  so  $d(j)$  divides the difference  $n_{ii}$ .
- (d) Now  $d(j)$  is a divisor of  $n_{ii}$  and  $d(i) = \gcd(n_{ii})$  so  $d(j) \leq d(i)$ .
- (e) By a symmetrical argument,  $d(i) \leq d(j)$  so  $d(i) = d(j)$ .
- (2) (a) For state  $i$ , let its equivalence class of communicating states be labeled  $1, \dots, k$ . For each state  $j$ ,  $1 \leq j \leq k$ , there is an  $m_{ij}$  such that  $(P^{m_{ij}})_{ij} > 0$  and an  $m_{ji}$  such that  $(P^{m_{ji}})_{ji} > 0$ .
- (b) Let  $n_j = m_{ij} + m_{ji}$ . Then

$$(P^{n_j})_{ii} = (P^{m_{ij}+m_{ji}})_{ii} \geq (P^{m_{ij}})_{ij}(P^{m_{ji}})_{ji} > 0.$$

That is, the probability of a return to  $i$  from  $i$  in  $n_j$  steps is at least as great as the probability of an excursion from  $i$  to  $j$  in  $m_{ij}$  steps with return to  $i$  from  $j$  in  $m_{ji}$  steps.

- (c) Using the Markov property of independence of the past and the future given the present state,  $(P^{n_j})_{ii} > 0$  implies that for any positive integer  $c_j$ ,  $(P^{c_j n_j})_{ii} > 0$ , that is, the probability of  $c_j$  sequential returns is still positive.
- (d) By the number theoretic Lemma 2.8, there exists  $N$  and positive integers  $c_1, \dots, c_k$  such that if  $n \geq N$

$$(P^{nd(i)})_{ii} = (P^{c_1 n_1 + \dots + c_k n_k})_{ii} \geq (P^{c_1 n_1})_{ii} \dots (P^{c_k n_k})_{ii} > 0.$$

- (3) Using the hypothesis

$$(P^{m+nd(i)})_{ji} \geq (P^{nd(i)})_{ii}(P^m)_{ji} > 0.$$

That is, the probability of an excursion to  $j$  from  $i$  in  $m + nd(i)$  steps is at least as great as the probability of an excursion from  $i$  to  $i$  in  $nd(i)$  steps followed by moving to  $j$  from  $i$  in  $m$  steps. By the previous part of the lemma, there is an  $N$  such that for  $n \geq N$ ,  $(P^{nd(i)})_{ii} > 0$  and so  $(P^{m+nd(i)})_{ji} > 0$  for sufficiently large  $n$ .

□

**Definition 2.9.** The Markov chain is **irreducible** if it has only one communicating class. In other words, a Markov chain is irreducible if all states communicate with each other. In turn this implies  $(P^m)_{ij} > 0$  for some  $m$  for all pairs of  $i$  and  $j$ . ◇

**Definition 2.10.** A Markov chain in which each state has period 1 is **aperiodic**. ◇

### 2.3. Recurrent and Transient States

**Definition 2.11.** Let the random variable  $\tau_{ij}$  be the **first passage time** to state  $j$  given the chain starts in  $i$ :

$$\begin{aligned} \tau_{ij} &= \min \{n \geq 1 : X_n = j \mid X_0 = i\} \\ \tau_{ij} &= \infty \text{ if } X_n \neq j, n \geq 1. \end{aligned}$$

◇

**Remark 2.12.** The first passage time to state  $j$  given the chain starts in  $i$  might also be called the *first visit time*. A frequent application is when  $j = i$  in which case the chain returns to  $i$ , so it is sometimes referred to as the first return time.

**Definition 2.13.** Let the distribution of  $\tau_{ij}$  be  $f_{ij}^n$ , the probability that starting from  $i$ , the first return to state  $j$  occurs at step  $n$ . That is, for each  $n \geq 1$ ,

$$f_{ij}^n = \mathbb{P}[X_n = j, X_\nu \neq i, \nu = 1, 2, \dots, n-1 \mid X_0 = i].$$

For convenience,  $f_{ij}^0 = 0$ . Note that  $f_{ij}^1 = P_{ij}$ .  $\diamond$

**Definition 2.14. Absorbing states** are a special case of states for which  $f_{ii}^1 = P_{ii} = 1$ .  $\diamond$

**Lemma 2.15.** *Recursively*  $f_{ij}^n = \sum_{\nu=0}^n f_{ij}^\nu (P^{\nu-k})_{jj}$ .

**Proof.** See the exercises.  $\square$

**Remark 2.16.** The recursive equation is an example of a *renewal equation*.

**Definition 2.17.** The **expected return time** is  $\mathbb{E}[\tau_{ii}] = m_i = \sum_{\nu=0}^{\infty} \nu f_{ii}^\nu$ .  $\diamond$

**Definition 2.18.** For any state  $i$ , let  $f_i = \mathbb{P}[\tau_{ii} < \infty] = \sum_{\nu=0}^{\infty} f_{ii}^\nu$  denote the probability that starting in  $i$  the process will *ever* reenter state  $i$ . State  $i$  is **recurrent** if  $f_i = 1$  and **transient** if  $f_i < 1$ .  $\diamond$

**Remark 2.19.** Note that the qualities of recurrence and transience are complementary, a state is one or the other, there are no other possibilities. If the state  $i$  is transient,  $f_i < 1$ , then  $i$  will be visited a finite random number of times. Starting from  $i$  the number of visits  $N_i$  (counting the starting visit) to transient state  $i$  has a geometric distribution

$$\mathbb{P}[N_i = n] = f_i^{n-1}(1 - f_i), n \geq 1.$$

This observation depends on the Strong Markov property, once the chain visits state  $i$ , the future is independent of the past and the chain starts over again with the same distribution. In fact, the expected number of visits is  $\mathbb{E}[N_i] = 1/(1 - f_i)$ .

**Proposition 2.20.** *If state  $i$  is recurrent, then with probability 1 the process will reenter  $i$  infinitely often.*

**Proof.** (1) Suppose that the process starts in state  $i$  and  $i$  is recurrent, so that with probability 1 the process will eventually reenter state  $i$ .  
 (2) However, by the definition of a Markov chain, it follows that the process will be starting over again when it reenters state  $i$ , and therefore state  $i$  will eventually be visited again.  
 (3) By induction, starting in state  $i$  will reenter state  $i$  any number of times, that is, infinitely often.  $\square$

**Proposition 2.21.** (1) *State  $i$  is recurrent if and only if*

$$\sum_{\nu=1}^{\infty} (P^\nu)_{ii} = \infty.$$

(2) State  $i$  is transient if and only if

$$\sum_{\nu=1}^{\infty} (P^{\nu})_{ii} < \infty.$$

**Proof.** (1) The two statements are complementary and equivalent so it suffices to prove the forward implication for each statement. First prove the statement for recurrence.

(2) Suppose  $i$  is recurrent, so by the previous Proposition the probability that starting from  $i$  the process will ever reenter  $i$  is 1 so the expected number of visits to  $i$  is infinite.

(3) That is,

$$\infty = \sum_{\nu=0}^{\infty} \mathbf{1}_{X_{\nu}=i|X_0=i} = \sum_{n=1}^{\infty} (P^n)_{ii}.$$

(4) Next prove the statement for transient. Suppose that state  $i$  is transient, so by definition  $f_i < 1$ . Let  $N_i$  count the total number of returns to  $i$ .

(5) Write  $N_i$  in terms of indicator variables as

$$N_i = \sum_{\nu=1}^{\infty} \mathbf{1}_{X_{\nu}=i}.$$

(6) The distribution of  $N_i$  is geometric with parameter  $f_i$  so

$$\mathbb{E}[N_i | X_0 = i] = \frac{f_i}{1 - f_i}.$$

Then

$$\infty > \mathbb{E}[N_i | X_0 = i] = \mathbb{E}\left[\sum_{n=1}^{\infty} \mathbf{1}_{X_n=i|X_0=i}\right] = \sum_{n=1}^{\infty} (P^n)_{ii}.$$

□

**Corollary 2.22.** (1) For any communication class  $C$  of a Markov chain, all states in  $C$  are either recurrent or all states in  $C$  are transient. That is

- if  $i$  and  $j$  communicate, and  $i$  is recurrent, then so is  $j$
- if  $i$  and  $j$  communicate, and  $i$  is transient, then so is  $j$ .

(2) For an irreducible Markov chain, either all states are recurrent or all states are transient.

**Proof.** Left as an exercise. □

## 2.4. Positive Recurrence

**Definition 2.23.** A state  $i$  is **positive recurrent** if it is recurrent and starting in  $i$ , the expected time until the process returns to state  $i$  is finite. Otherwise the state is **null recurrent**. ◇

**Definition 2.24.** Let the random variable  $\tau_{ij}$  be the **first passage time** to state  $j$  given the chain starts in  $i$ :

$$\begin{aligned}\tau_{ij} &= \min \{n \geq 1 : X_n = j \mid X_0 = i\} \\ \tau_{ij} &= \infty \text{ if } X_n \neq j, n \geq 1.\end{aligned}$$

◇

**Proposition 2.25.** *Suppose states  $i, j$  are both recurrent. If  $i$  and  $j$  communicate and if  $j$  is positive recurrent,  $\mathbb{E}[\tau_{jj}] < \infty$ , then  $i$  is positive recurrent and furthermore  $\mathbb{E}[\tau_{ij}] < \infty$ . In particular, all states in a recurrent communicating class are either all positive recurrent or all null recurrent.*

**Proof.** (1) Assume  $\mathbb{E}[\tau_{jj}] < \infty$  and  $i$  and  $j$  communicate.

- (2) Choose the smallest  $n \geq 1$  such that  $(P^n)_{ji} > 0$ .
- (3) With  $x_0 = j$ , let  $A = \{x_l \neq j, 1 \leq l < n, x_n = i\}$  be a specific path of states visited from  $j$  to  $i$ . Note that  $\mathbb{P}[A] > 0$ .
- (4) Then  $\mathbb{E}[\tau_{jj}] \geq \mathbb{E}[\tau_{jj} \mid A] \cdot \mathbb{P}[A] = (n + \mathbb{E}[\tau_{ij}]) \cdot \mathbb{P}[A]$ . Hence  $\mathbb{E}[\tau_{ij}] < \infty$ .
- (5) With  $x_0 = j$ , let  $\{Y_m : m \geq 1\}$  be the interarrival times between visits to state  $j$ . The distribution of  $Y_m$  is the same as the distribution of  $\tau_{jj}$ . The  $n$ th revisit of the chain to state  $j$  is at time  $t_n = Y_1 + \cdots + Y_n$  with  $\mathbb{E}[Y_l] = \mathbb{E}[\tau_{jj}] < \infty$ .
- (6) Let  $p$  be the probability the chain visits state  $i$  before returning to state  $j$ , given that the chain started in  $j$ . Then  $p \geq \mathbb{P}[A] > 0$  where  $A$  is defined in step 3.
- (7) Every time the chain revisits state  $j$ , there is, independent of the past, probability  $p$  that the chain will visit state  $i$  before revisiting state  $j$  again. Letting  $N$  denote the number of revisits the chain makes to state  $j$  until first visiting state  $i$ ,  $N$  has geometric distribution with “success” probability  $p$  and so  $\mathbb{E}[N] < \infty$ .
- (8)  $N$  is a stopping time with respect to the  $\{Y_m\}$  and

$$\tau_{ji} \leq \sum_{m=1}^N Y_m$$

and so by Wald’s equation  $\mathbb{E}[\tau_{ji}] \leq \mathbb{E}[N] \cdot \mathbb{E}[Y] < \infty$ .

- (9) Finally,  $\mathbb{E}[\tau_{ii}] \leq \mathbb{E}[\tau_{ij}] + \mathbb{E}[\tau_{ji}] < \infty$ .

□

**Proposition 2.26.** *In an irreducible finite-state Markov chain all recurrent states are positive recurrent.*

**Proof.** (1) If the state space is finite, then not *all* states can be transient. Otherwise, after a finite number of steps, the chain would leave every state never to return, clearly an impossibility. That is, all the communicating states are recurrent.

- (2) Now show that state  $i$  can’t be null recurrent, that is, it must be positive recurrent.



(3) For any fixed  $m \geq 1$ , the rows of  $P^m$  must sum to 1. That is, for any  $i \in \mathcal{X}$

$$\sum_{j \in \mathcal{X}} (P^m)_{ij} = 1.$$

(4) Suppose the state is null recurrent, then for any  $j \in \mathcal{X}$ .

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n (P^\nu)_{ij} = 0.$$

(5) Summing over  $j$

$$\sum_{j \in \mathcal{X}} \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n (P^\nu)_{ij} = 0.$$

(6) Since the state space is finite, interchange the outer sum and the limit.

$$\lim_{n \rightarrow \infty} \sum_{j \in \mathcal{X}} \frac{1}{n} \sum_{\nu=1}^n (P^\nu)_{ij} = 0.$$

(7) Interchange the order of summation,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n \sum_{j \in \mathcal{X}} (P^\nu)_{ij} = 0.$$

(8) But

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n \sum_{j \in \mathcal{X}} (P^\nu)_{ij} = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n 1 = \lim_{n \rightarrow \infty} \frac{1}{n} \cdot n = 1,$$

a contradiction.

(9) Thus, the state must be positive recurrent. □

**Definition 2.27.** Positive recurrent and aperiodic states are **ergodic**. ◇

**Remark 2.28.** This text does not use the term *ergodic*. Instead the fully descriptive terms *positive recurrent* and *aperiodic* emphasize the state properties.

**Example 2.29.** In infinite state space Markov chains recurrence, transience, positive recurrence and null recurrence are distinct. Symmetric nearest neighbor random walk on  $\mathbb{Z}$  and  $\mathbb{Z}^2$  is null recurrent. However symmetric nearest neighbor random walk on  $\mathbb{Z}^n$  for  $n \geq 3$  is transient. See [Les05, Chapter 13] ▽

## 2.5. Fundamental Theorems for Markov Chains

**Remark 2.30.** Make the notation convention that  $(P^0)_{ii} = 1$ . Recall the definition of the **expected return time** as  $m_i = \mathbb{E}[\tau_{ii}] = \sum_{\nu=0}^{\infty} \nu f_{ii}^\nu$ .

**Lemma 2.31.** (1) Let  $a_n, u_n, b_n$  be sequences for  $n \geq 0$ .

(2)  $a_n \geq 0$ ,  $a_1 > 0$ , and  $\sum_{\nu=0}^{\infty} a_\nu = 1$ .

(3) The greatest common divisor of the integers  $n$  for which  $a_n > 0$  is 1.

(4)  $b_n \geq 0$  and  $b_n \rightarrow 0$  as  $n \rightarrow \infty$ .

(5) The renewal equation

$$u_n - \sum_{\nu=0}^n a_{n-\nu} u_\nu = b_n$$

is satisfied by a bounded sequence  $u_n$ .

Then

$$\lim_{n \rightarrow \infty} u_n = \frac{\sum_{\nu=0}^{\infty} b_\nu}{\sum_{\nu=0}^{\infty} \nu a_\nu}.$$

**Proof.** (1) Hypothesis 2 implies  $0 \leq a_0 < 1$ .

(2) Changing the variable of summation, the renewal equation is equivalent to

$$u_n - \sum_{\nu=0}^n a_\nu u_{n-\nu} = b_n.$$

(3) For  $n = 0$ , the renewal equation is  $u_0 - a_0 u_0 = b_0$ . Using hypotheses 2 and 4,  $u_0 \geq 0$ . Inductively,

$$u_n - a_0 u_n - \sum_{\nu=1}^n a_\nu u_{n-\nu} = b_n$$

so  $u_n \geq 0$ .

(4) By hypothesis 5,  $u_n$  is a bounded sequence, so  $\lambda = \limsup_{n \rightarrow \infty} u_n < \infty$ . Let  $n_1 < n_2 < \dots$  be a subsequence along which  $\lim_{j \rightarrow \infty} u_{n_j} = \lambda$ . The claim is that  $\lim_{j \rightarrow \infty} u_{n_j-1} = \lambda$  by using  $a_1 > 0$  from hypothesis 2.

(5) Proof of the claim by contradiction.

(a) Suppose  $\lim_{j \rightarrow \infty} u_{n_j-1} \neq \lambda$ . Then there is  $\lambda' < \lambda$  such that  $u_{n_j-1} < \lambda'$  for infinitely many  $j$ . Use  $\epsilon = a_1(\lambda - \lambda')/4$ ,  $M = \sup_{\nu \geq 0} u_\nu$ , and  $N$  so large that  $\sum_{\nu=0}^n a_\nu > 1 - \epsilon/M$  for  $n > N$ . Let  $j$  be large enough that  $n_j > N$  and  $u_{n_j} > \lambda - \epsilon$ ,  $u_{n_j-1} < \lambda' < \lambda$ ,  $0 \leq b_{n_j} < \epsilon$  and  $u_n < \lambda + \epsilon$  for  $n > n_j - N$ .

(b) Then

$$\begin{aligned} u_{n_j} &\leq \sum_{\nu=0}^{n_j} a_\nu u_{n_j-\nu} + \epsilon \\ &< \sum_{\nu=0}^N a_\nu u_{n_j-\nu} + M \sum_{\nu=N+1}^{n_j} a_k + \epsilon \\ &< \sum_{\nu=0}^N a_\nu u_{n_j-\nu} + 2\epsilon \\ &< (a_0 + a_2 + \dots + a_N)(\lambda + \epsilon) + a_1 \lambda' + 2\epsilon \\ &< (1 - a_1)(\lambda + \epsilon) + a_1 \lambda' + 2\epsilon \\ &< \lambda + 3\epsilon - a_1(\lambda - \lambda') \\ &= \lambda - \epsilon. \end{aligned}$$

(c) The inequality from the previous step contradicts  $u_{n_j} > \lambda - \epsilon$  and the claim is established,  $\lim_{j \rightarrow \infty} u_{n_j-1} = \lambda$ .

- (6) Repeating the argument for  $d \geq 0$ ,  $\lim_{j \rightarrow \infty} u_{n_j-d} = \lambda$ .
- (7) Let  $r_n = \sum_{\nu=n+1}^{\infty} a_\nu$ . Then by summation by parts,  $\sum_{\nu=0}^{\infty} ka_k = \sum_{\nu=0}^{\infty} r_n$ . No assumption is made about the convergence of  $\sum_{\nu=0}^{\infty} ka_k = \sum_{\nu=0}^{\infty} r_n$ . Note that  $a_n = r_{n-1} - r_n$  for  $n \geq 1$ . Also note that  $r_0 = 1 - a_0$ .
- (8) Starting with the renewal equation in the form

$$u_n - a_0 u_n - a_1 u_{n-1} - \cdots - a_n u_0 = b_n$$

and substituting  $-a_\nu = r_\nu - r_{\nu-1}$  gives

$$u_n - a_0 u_n + (r_1 - r_0)u_{n-1} + \cdots + (r_n - r_{n-1})u_0 = b_n.$$

Rearranging and using  $r_0 = 1 - a_0$

$$r_0 u_n + r_1 u_{n-1} + \cdots + r_n u_0 = r_0 u_{n-1} + r_1 u_{n-2} + \cdots + r_{n-1} u_0 + b_n.$$

- (9) Set  $A_n = r_0 u_n + \cdots + r_n u_0$ , the previous equation becomes  $A_n = A_{n-1} + b_n$  with  $A_0 = r_0 u_0 = (1 - a_0)u_0 = b_0$ . Then  $A_n = \sum_{\nu=0}^n b_\nu$ .
- (10) Since  $r_n \geq 0$  and  $u_n \geq 0$ , for any  $N > 0$  and  $j > 0$

$$r_0 u_{n_j} + r_1 u_{n_j-1} + \cdots + r_N u_{N_j-N} \leq A_{n_j} = \sum_{\nu=0}^{n_j} b_\nu.$$

- (11) Letting  $j \rightarrow \infty$  gives

$$(r_0 + \cdots + r_N)\lambda \leq \sum_{\nu=0}^{\infty} b_\nu$$

or equivalently  $\lambda \leq \sum_{\nu=0}^{\infty} b_\nu / \sum_{\nu=0}^N r_\nu$ .

- (12) Since  $N > 0$  is arbitrary,  $\lambda \leq \sum_{\nu=0}^{\infty} b_\nu / \sum_{\nu=0}^{\infty} r_\nu$ .
- (13) Since  $u_n \geq 0$  for all  $n$ , this proves the theorem in the case  $\sum_{\nu=0}^{\infty} ka_k = \sum_{\nu=0}^{\infty} r_n = \infty$  since then  $\lambda = \lim_{n \rightarrow \infty} u_n = 0$ .
- (14) If  $\sum_{\nu=0}^{\infty} r_n < \infty$ , let  $\mu = \liminf_{n \rightarrow \infty} u_n$ . As in step 5, then  $\lim_{j \rightarrow \infty} u_{n_j-d} = \mu$  for each integer  $d$ . (See the exercises for a proof.)
- (15) Set  $g_N = \sum_{\nu=N+1}^{\infty} r_n$  so  $\lim_{N \rightarrow \infty} g_N = 0$  and

$$\sum_{\nu=0}^{n_j} b_\nu \leq r_0 u_{n_j} + r_1 u_{n_j-1} + \cdots + r_N u_{N_j-N} + g_N \cdot M.$$

- (16) Letting  $j \rightarrow \infty$

$$\sum_{\nu=0}^{n_j} b_\nu \leq (r_0 + r_1 + \cdots + r_N)\mu + g_N \cdot M$$

and taking the limit as  $N \rightarrow \infty$

$$\sum_{\nu=0}^{\infty} b_\nu \leq \mu \sum_{\nu=0}^{\infty} r_\nu$$

or  $\mu \geq \sum_{\nu=0}^{\infty} b_\nu / \sum_{\nu=0}^{\infty} r_\nu$ .

(17) Steps 11 and 16 imply  $\mu \geq \lambda$  which means  $\mu = \lambda = \lim_{n \rightarrow \infty} u_n$  with value

$$\lim_{n \rightarrow \infty} u_n = \sum_{\nu=0}^{\infty} b_{\nu} \bigg/ \sum_{\nu=0}^{\infty} r_{\nu}.$$

□

**Remark 2.32.** Recall that the expected return time is  $m_i = \sum_{\nu=1}^{\infty} \nu f_{ii}^{\nu}$ .

**Theorem 2.33** (Power Limit as Reciprocal Mean Return Time). *For an irreducible, recurrent, and aperiodic Markov chain,*

$$\lim_{n \rightarrow \infty} (P^n)_{ii} = \frac{1}{m_i}.$$

**Proof.** (1) The renewal equation for the transition probabilities is

$$(P^n)_{ii} - \sum_{\nu=0}^n f_{ii}^{n-\nu} (P^{\nu})_{ii} = \begin{cases} 1 & n = 0, \\ 0 & n > 0. \end{cases}$$

(2) Using the previous Lemma, identify  $u_n = (P^n)_{ii}$ ,  $a_n = f_{ii}^n$ ,  $b_0 = 1$ ,  $b_n = 0$  for  $n > 0$ .

(3) Then

$$\begin{aligned} \lim_{n \rightarrow \infty} u_n &= \sum_{\nu=0}^{\infty} b_{\nu} \bigg/ \sum_{\nu=0}^{\infty} r_{\nu} \\ &= 1 \bigg/ \sum_{\nu=0}^{\infty} \nu f_{ii}^{\nu} \\ &= 1/m_i. \end{aligned}$$

□

**Theorem 2.34** (Limit Theorem for Transition Matrix Powers). *For positive recurrent aperiodic states  $i, j$*

$$\lim_{n \rightarrow \infty} (P^n)_{ji} = \lim_{n \rightarrow \infty} (P^n)_{ii}.$$

**Proof.** (1) Start with the recursion relation

$$(P^n)_{ji} = \sum_{\nu=0}^n f_{ji}^{\nu} (P^{n-\nu})_{ii}$$

for  $i \neq j$  and  $n \geq 0$ .

(2) Change the order of summation

$$(P^n)_{ji} = \sum_{\nu=0}^n f_{ji}^{n-\nu} (P^{\nu})_{ii}$$

for  $i \neq j$  and  $n \geq 0$ .

(3) More generally, consider the convolution type relation

$$y_n = \sum_{\nu=0}^n a_{n-\nu} x_\nu$$

where  $a_n \geq 0$ ,  $\sum_{\nu=0}^{\infty} a_\nu = 1$ , and  $\lim_{\nu \rightarrow \infty} x_\nu = c$ . The goal is to prove that  $\lim_{n \rightarrow \infty} y_n = c$ .

(4) Take the difference with  $c$  and break into sums from 0 to  $n$  and  $n+1$  to  $\infty$

$$y_n - c = \sum_{\nu=0}^n a_{n-\nu} x_\nu - c \sum_{\nu=0}^{\infty} a_\nu = \sum_{\nu=0}^n a_{n-\nu} (x_\nu - c) - c \sum_{\nu=n+1}^{\infty} a_\nu.$$

(5) Let  $\epsilon > 0$  be given and determine  $N(\epsilon)$  so that  $|x_\nu - c| < \epsilon/3$  for  $\nu \geq N(\epsilon)$ . For  $n \geq N(\epsilon)$

$$y_n - c = \sum_{\nu=0}^{N(\epsilon)} a_{n-\nu} (x_\nu - c) + \sum_{\nu=N(\epsilon)+1}^n a_{n-\nu} (x_\nu - c) - c \sum_{\nu=n+1}^{\infty} a_\nu.$$

(6) Let  $M = \max_{1 \leq \nu \leq N(\epsilon)} \{|x_\nu - c|\}$ , so by the Triangle Inequality

$$|y_n - c| \leq M \sum_{\nu=0}^{N(\epsilon)} a_{n-\nu} + \frac{\epsilon}{3} \sum_{\nu=N(\epsilon)+1}^n a_{n-\nu} + |c| \sum_{\nu=n+1}^{\infty} a_\nu.$$

(7) If necessary, increase  $N(\epsilon)$  so that  $|c| \sum_{\nu=n+1}^{\infty} a_\nu \leq \epsilon/3$  and

$$\sum_{\nu=0}^{N(\epsilon)} a_{n-\nu} = \sum_{\nu=n-N(\epsilon)}^n a_\nu \leq \frac{\epsilon}{3M}$$

for  $n \geq N(\epsilon)$ .

(8) Summarizing, for  $n \geq N(\epsilon)$ ,  $|y_n - c| \leq \epsilon/3 + \epsilon/3 + \epsilon/3 = \epsilon$ .

(9) Using the hypotheses and the Power Limit as Reciprocal Mean Return Time Theorem,  $\lim_{n \rightarrow \infty} (P^n)_{ii}$  exists. Applying this to  $y_n = (P^n)_{ji}$ ,  $a_n = f_{ji}^n$ ,  $x_n = (P^n)_{ii}$  gives the final result.  $\square$

**Remark 2.35.** This proof is a purely analytic result with the probabilistic application due to the assumption that  $\sum_{\nu=0}^{\infty} a_\nu = 1$ .

**Lemma 2.36.** If  $a_n \rightarrow a$  as  $n \rightarrow \infty$ , then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n a_\nu = a,$$

so that if  $a_n$  converges to  $a$ , the sequence of averages converges to  $a$ .

**Proof.** Left as an exercise.  $\square$

**Definition 2.37.** When the limit exists, let

$$\pi_j = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n \mathbf{1}_{X_\nu=j|X_0=i}$$

denote the **long run proportion of time the chain spends in state  $j$**  or just the *long run proportion* for short. Note that the right side appears to depend on the starting state  $i$ , but the Limit Theorem shows that the long run proportion is independent of  $i$ .  $\diamond$

**Corollary 2.38** (Long Run Proportion as Reciprocal Mean Return Time).

$$\pi_i = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n (P^\nu)_{ii} = \frac{1}{\sum_{\nu=0}^{\infty} \nu f_{ii}^\nu} = \frac{1}{m_i},$$

**Remark 2.39.** Taking expected values,

$$\mathbb{E} [\mathbf{1}_{X_m=j} | X_0=i] = \mathbb{P} [X_m = j | X_0 = i] = (P^m)_{ij}$$

so using the Limit Theorem for Transition Matrix Powers, the long run proportion is alternatively defined as

$$\pi_j = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n (P^\nu)_{ij}$$

independently of  $i$ . This remark uses the Bounded Convergence Theorem to interchange the limit and the expectation.

**Remark 2.40.** Recalling that  $(P^\nu)_{ij}$  is the  $i, j$  component of the matrix  $P^\nu$  and using the independence on  $i$ , the long run proportions in matrix form are

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n P^\nu = \begin{pmatrix} \pi_1 & \pi_2 & \dots & \pi_k \\ \pi_1 & \pi_2 & \dots & \pi_k \\ \vdots & \vdots & \ddots & \vdots \\ \pi_1 & \pi_2 & \dots & \pi_k \end{pmatrix} = \begin{pmatrix} \boldsymbol{\pi} \\ \boldsymbol{\pi} \\ \vdots \\ \boldsymbol{\pi} \end{pmatrix}.$$

**Remark 2.41.** Observing the Markov chain at a time far in the future,  $\pi_j$  is approximately the probability the chain is in state  $j$ . To see this: Let  $N$  be a random observation time, with uniform distribution over the integers  $\{1, 2, \dots, n\}$ , independent of the chain. Then conditioning on  $N$

$$\mathbb{P} [X_N = j] = \sum_{\nu=1}^n \mathbb{P} [X_\nu = j | X_0 = i] \mathbb{P} [N = \nu] = \frac{1}{n} \sum_{\nu=1}^n (P^\nu)_{ij} \approx \pi_j.$$

**Theorem 2.42** (Fundamental Theorem of Markov Chains). *For an irreducible, positive recurrent and aperiodic Markov chain  $\lim_{n \rightarrow \infty} (P^n)_{ij}$  exists and is independent of  $i$ . Furthermore, letting*

$$\pi_j = \lim_{n \rightarrow \infty} (P^n)_{ij}$$

*then  $\pi_j$  is the unique nonnegative solution of*

$$(2.1) \quad \sum_i \pi_i P_{ij} = \pi_j,$$

$$(2.2) \quad \sum_i \pi_i = 1.$$

**Proof.** (1) First,  $\pi_j = \lim_{n \rightarrow \infty} (P^n)_{ij}$  exists and is independent of  $i$  by the Limit Theorem for Transition Matrix Powers.

- (2) Recall  $k$  is the number of states in the Markov chain, possibly  $k = \infty$ .  
 (3) For every  $n$  and  $M \leq k$ ,  $1 = \sum_{j=0}^k (P^n)_{ij} \geq \sum_{j=0}^M (P^n)_{ij}$ .  
 (4) Letting  $n \rightarrow \infty$ , the limit exists so  $1 \geq \sum_{j=0}^M \pi_j$  for every  $M$ . Thus,  $1 \geq \sum_{j=0}^k \pi_j$ .  
 (5) Now  $(P^{n+1})_{ij} \geq \sum_{\nu=0}^M (P^n)_{i\nu} P_{\nu j}$ . Again let  $n \rightarrow \infty$  to obtain

$$\pi_j \geq \sum_{\nu=0}^M \pi_\nu P_{\nu j}.$$

- (6) Since the left side is independent of  $M$ , let  $M \rightarrow k$  giving

$$\pi_j \geq \sum_{\nu=0}^k \pi_\nu P_{\nu j}.$$

- (7) Multiply by  $P_{ji}$ , sum on  $j$ , and use the previous step to assert

$$\pi_i > \pi_j P_{ji} \geq \sum_{\nu=0}^{\infty} \pi_\nu (P^2)_{\nu i}.$$

Then by induction and renaming the state index from  $i$  back to  $j$

$$\pi_j \geq \sum_{\nu=0}^{\infty} \pi_\nu (P^n)_{\nu j}.$$

- (8) In the previous inequality, suppose strict inequality holds for some  $j$ , then add over  $j$

$$\sum_{j=0}^k \pi_j > \sum_{j=0}^k \sum_{\nu=0}^{\infty} \pi_\nu (P^n)_{\nu j} = \sum_{\nu=0}^{\infty} \pi_\nu \sum_{j=0}^k (P^n)_{\nu j} = \sum_{j=0}^k \pi_j$$

which is a contradiction. Thus

$$\pi_j = \sum_{j=0}^k \pi_j (P^n)_{jj}.$$

- (9) Let  $n \rightarrow \infty$ , and use that  $\sum \pi_\nu$  converges and  $(P^n)_{\nu j}$  is uniformly bounded to conclude

$$\pi_j = \sum_{\nu=0}^{\infty} \pi_\nu \lim_{n \rightarrow \infty} (P^n)_{\nu j} = \pi_j \sum_{\nu=0}^{\infty} \pi_\nu$$

for every  $j$ . Thus  $\sum_{\nu=0}^{\infty} \pi_\nu = 1$  since  $\pi_j > 0$  by positive recurrence.

- (10) Now suppose  $x = \{x_n\}$  satisfies equations 2.1 and 2.2. Then as before

$$x_j \geq \sum_{\nu=0}^k x_\nu (P^n)_{\nu j}.$$

Let  $n \rightarrow \infty$  as before to see that

$$x_j = \sum_{\nu=0}^k x_\nu (P^n)_{\nu j} = \pi_k \sum_{\nu=0}^k x_j = \pi_k.$$

□

**Definition 2.43.** Any vector  $(\pi_j)$  satisfying equations 2.1 and 2.2 is a **stationary probability distribution** of the Markov chain. A Markov chain started according to a stationary distribution  $(\pi_j)$  will have this distribution for all future times.  $\diamond$

**Remark 2.44.** A limiting distribution is always a stationary distribution, but the converse is not true. A Markov chain may have a stationary distribution but no limiting distribution. For example, the periodic Markov chain whose transition probability matrix is

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

has no limiting distribution but  $\pi = (1/2, 1/2)$  is a stationary distribution. Notice that this Markov chain is not aperiodic so it fails to satisfy the requirements of the Fundamental Theorem.

**Remark 2.45.** The Fundamental Theorem says that a transition probability matrix for an irreducible, positive recurrent, and aperiodic Markov chain has a *left* eigenvector with corresponding eigenvalue 1. This is a special case of the more general Perron-Frobenius Theorem.

**Remark 2.46.** The Fundamental Theorem says that under appropriate conditions, the powers of the transition probability matrix converge to the stationary distribution but gives no information about the rate of convergence. The following theorem gives a first indication about the rate of convergence.

**Theorem 2.47** (Convergence Theorem by Total Variation). *Suppose that  $P$  is the transition probability matrix for an irreducible and aperiodic Markov chain with stationary distribution  $\pi$ . Then there exist constants  $\alpha \in (0, 1)$  and  $C > 0$  such that*

$$\max_{x \in \mathcal{X}} \|(P^n)_i - \pi\|_{TV} \leq C\alpha^n.$$

**Proof.** (1) Since  $P$  is irreducible and aperiodic, there exist  $r$  such that  $P^r$  has strictly positive entries.

(2) Let  $\Pi$  be the matrix with  $\text{card}(\mathcal{X}) = k$  rows, each of which is the row vector  $\pi$ .

(3) For sufficiently small  $\delta > 0$ ,  $(P^r)_{ij} \geq \delta\pi_j$  for  $i, j \in \mathcal{X}$ .

(4) Let  $\theta = 1 - \delta$ . Define stochastic matrix  $Q$  by

$$P^r = (1 - \theta)\Pi + \theta Q.$$

(5) Note that  $M\Pi = \Pi$  for any stochastic matrix and  $\Pi M = \Pi$  for any matrix with  $\pi M = \pi$ .

(6) Claim:

$$P^{rn} = (1 - \theta^n)\Pi + \theta^n Q^n.$$

Proof by Induction: For  $n = 1$ , this is the definition of  $Q$ . Assume the claim is true for  $n$ .

$$\begin{aligned} P^{r(n+1)} &= P^{rn} P^r = [(1 - \theta^n)\Pi + \theta^n Q^n] P^r \\ &= (1 - \theta^n)\Pi P^r + (1 - \theta)\theta^n Q^n \Pi + \theta^{n+1} Q^n Q. \end{aligned}$$



Use  $\Pi P^r = \Pi$  and  $Q^n \Pi = \Pi$ .

$$P^{r(n+1)} = (1 - \theta^{n+1})\Pi + \theta^{n+1}Q^{n+1}.$$

Hence the relation holds for all  $n$ .

- (7) Multiply by  $P^j$ , and rearrange to obtain

$$P^{rn+j} - \Pi = \theta^n(Q^n P^j - \Pi).$$

- (8) Sum the absolute value of row  $\nu$  on both sides and divide by 2. On the right, the absolute row- $\nu$  sum from  $(Q^n P^j - \Pi)$  is at most the largest possible total variation distance between distributions (which is at most 1). Hence

$$\|(P^{rn+j})_{\cdot} - \pi\|_{TV} \leq \theta^n.$$

- (9) To finish the proof, let  $\alpha = \theta^{1/r}$  and  $C = 1/\theta$ .

□

## 2.6. Amusing Example of a Stationary Distribution

This finite state Markov chain has interest partly in the humorous context and partly that the context obscures that the Markov chain has more states than is at first obvious. It is also similar to a more serious application, a finite state machine, an abstract machine that can be in exactly one of a finite number of states at any given time. The finite state machine can change from one state to another in response to some inputs. Alternatively, this is an example of a random walk on a graph, illustrated in Figure 2.1.

There is a bathroom in your office building that has only one toilet. There is a small sign stuck to the outside of the door that you can slide from “Vacant” to “Occupied” so that no one else will try the door handle (theoretically) when you are inside. Unfortunately, people often forget to slide the sign to “Occupied” when entering, and they often forget to slide it to “Vacant” when exiting.

Assume that  $1/3$  of bathroom users don’t notice the sign upon entering or exiting. Therefore, whatever the sign reads before their visit, it still reads the same thing during and after their visit. Another  $1/3$  of the users notice the sign upon entering and make sure that it says “Occupied” as they enter. However, half the time they forget to slide it to “Vacant” when they exit. The remaining  $1/3$  of the users are very conscientious: They make sure the sign reads “Occupied” when they enter, and then they slide it to “Vacant” when they exit. Finally, assume that the bathroom is occupied exactly half of the time, all day, every day.

Two questions about this workplace situation:

- (1) If you go to the bathroom and see that the sign on the door reads “Occupied,” what is the probability that the bathroom is actually occupied?
- (2) If the sign reads “Vacant,” what is the probability that the bathroom actually is vacant?

- (3) Extra credit: What happens as the percentage of conscientious bathroom users changes?

The first step defines the states and transition probabilities. Because the bathroom can be either *occupied* or *vacant*, and the sign in front can either read “Vacant” or “Occupied”, there are at least four states, one for each possible pair of occupation state and sign. However, consider the state “bathroom is occupied and the sign says it’s occupied”. The states must distinguish between the cases where the person occupying the bathroom is conscientious (they will definitely slide the sign to “Vacant” when they leave) or not (they might leave the sign as “Occupied” after they leave).

Imagine a sequence of short times, say every minute. Using the assumption that the bathroom is occupied exactly half of the time, all day, every day, the transition from state to state each minute is a Markov chain with transition probability

$$\begin{array}{c} O \quad V \\ O \left( \begin{array}{cc} 1/2 & 1/2 \\ 1/2 & 1/2 \end{array} \right) \\ V \end{array}$$

It is easy to see that this chain is irreducible, positive recurrent and aperiodic. The stationary distribution is  $(1/2, 1/2)$ , consistent with the assumption that the bathroom is occupied exactly half of the time, all day, every day.

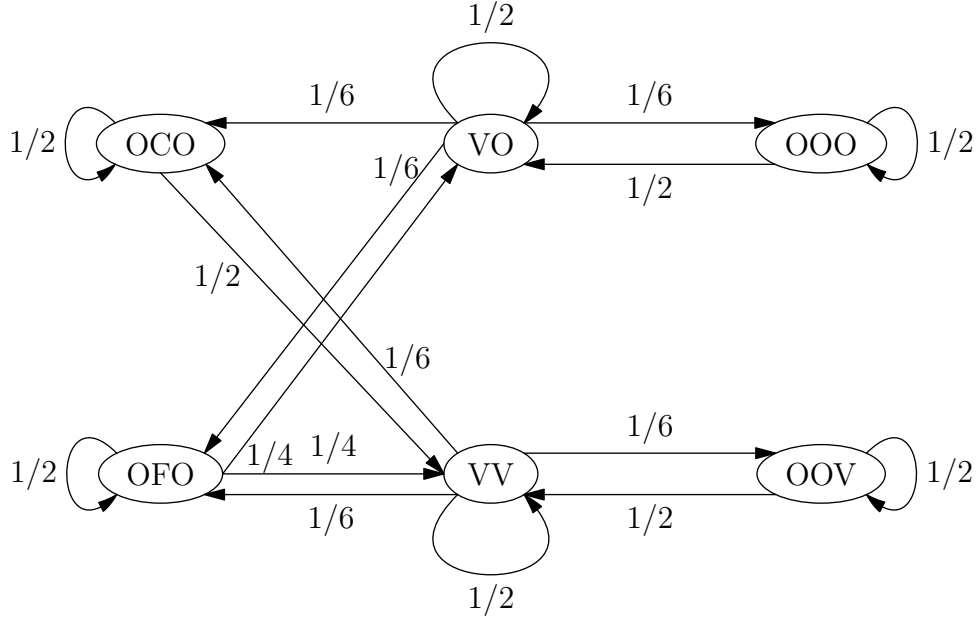
Augment the states to the Markov chain corresponding to the different ways in which the bathroom can be occupied. There are three types of users: oblivious, forgetful, and conscientious, each of proportion  $1/3$  and 4 combinations of occupation status and outside sign. There are 12 possible states but some will not occur because of the user habits.

Referring to Figure 2.1 the possible transitions at each minute are:

- (1) A Conscientious person is in the bathroom, and it is Occupied and the sign says Occupied. This state is *OCO*. Either the person stays and the state remains Occupied with sign Occupied with probability  $1/2$ , or the conscientious person leaves and the state is *VV* with probability  $1/2$ .
- (2) A Forgetful person is in the bathroom, and it is Occupied and the sign says Occupied. This state is *OFO*. Either the person stays and the state remains Occupied with sign Occupied with probability  $1/2$ , or the forgetful person leaves and the state is *VO* with probability  $1/2 \cdot 1/2 = 1/4$  or the forgetful person leaves, changing the sign and the state is *VV* with probability  $1/2 \cdot 1/2 = 1/4$ .
- (3) An Oblivious person is in the bathroom, and it is Occupied and the sign says Occupied. Name this state as *OOO*. Either the person stays and the state remains Occupied with sign Occupied with probability  $1/2$ , or the oblivious person leaves and the state is *VO* with probability  $1/2$ .
- (4) A Oblivious person is in the bathroom, and it is Occupied but the sign says Vacant. Name this state as *OOV*. Either the person stays and the state remains Occupied with sign Vacant with probability  $1/2$ , or the oblivious person leaves and the state is *VV* with probability  $1/2$ .

- (5) The bathroom is Vacant, but the sign says Occupied. With probability  $1/2$  some person will approach, nevertheless try the door and find the true state of vacancy and enter, dealing with the sign according to their type. Then the transition is to  $OCO$  with probability  $1/6$ ,  $OFO$  with probability  $1/6$  and  $OOO$  with probability  $1/6$ . With probability  $1/2$  the state remains  $VO$ .
- (6) The bathroom is Vacant, and the sign says Vacant. With probability  $1/2$  some person will approach, nevertheless try the door and easily find the true state of vacancy and enter, dealing with the sign according to their type. Then the transition is to  $OCO$  with probability  $1/6$ ,  $OFO$  with probability  $1/6$  and  $OOV$  with probability  $1/6$ . With probability  $1/2$  the state remains  $VV$ .

A state transition diagram is in Figure 2.1.



**Figure 2.1.** The state transition diagram for bathroom occupancy.

Then the transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & 1/2 \\ 0 & 1/2 & 0 & 0 & 1/4 & 1/4 \\ 0 & 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ 1/6 & 1/6 & 1/6 & 0 & 1/2 & 0 \\ 1/6 & 1/6 & 0 & 1/6 & 0 & 1/2 \end{pmatrix} \end{pmatrix}.$$

From Figure 2.1 it is easy to see that the chain is irreducible and recurrent. Because of the self-loops the states are aperiodic. The stationary distribution is

then the solution of

$$\pi P = \pi, \quad \sum_i \pi_i = 1$$

with solution

$$\begin{aligned} \pi_{OCO} &= \frac{1}{6}, & \pi_{OFO} &= \frac{1}{6}, & \pi_{OOO} &= \frac{1}{12}, \\ \pi_{OOV} &= \frac{1}{12}, & \pi_{VO} &= \frac{1}{4}, & \pi_{VV} &= \frac{1}{4}. \end{aligned}$$

Note that the bathroom is still Vacant half the time, although the time splits equally over the 2 sign states.

$$\begin{aligned} \mathbb{P}[\text{Vacant} \mid \text{says "Vacant"}] &= \frac{\pi_{VV}}{\pi_{VV} + \pi_{OOV}} = \frac{1/4}{1/4 + 1/12} = \frac{3}{4}, \\ \mathbb{P}[\text{Occupied} \mid \text{says "Occupied"}] &= \frac{\pi_{OCO} + \pi_{OFO} + \pi_{OOO}}{\pi_{OCO} + \pi_{OFO} + \pi_{OOO} + \pi_{VO}} = \frac{5}{8}. \end{aligned}$$

## 2.7. Example on an Infinite State Space

Consider a random walk restricted to the nonnegative integers. Here  $P_{0,1} = 1$  and otherwise,  $P_{i,i-1} = p$  with  $p > 1/2$  and  $P_{i,i+1} = 1 - p < 1/2$ . The restriction  $p > 1/2$  insures that a stationary distribution exists. The equations for stationarity are

$$\pi_0 = p\pi_1, \quad \pi_1 = \pi_0 + p\pi_2, \quad \pi_i = (1-p)\pi_{i-1} + p\pi_{i+1} \quad i \geq 2.$$

together with the normalization condition  $\sum_{\nu=0}^{\infty} \pi_{\nu} = 1$ . The solution is the stationary distribution  $\pi_0 = \frac{2p-1}{2p}$  and  $\pi_{\nu} = \frac{2p-1}{2p} \left( \frac{(1-p)^{\nu-1}}{p^{\nu}} \right)$  for  $\nu \geq 1$ . (See the exercises.)

This Markov chain can be interpreted as random walk with negative drift and reflecting boundary on the nonnegative integers. It can also be interpreted as the embedded discrete-time chain for an M/M/1 queue in which  $p = \frac{s}{r+s}$  where  $r$  is the arrival rate of customers and  $s$  is the service rate.

## 2.8. Chapter Ending Answer

Because the urns are labeled arbitrarily, there is no reason to believe that the fraction of time urn  $A$  is empty depends how the balls are initially distributed between the two urns. The randomizing of urn selection should also quickly remove any initial information, so again there is no reason to believe that the fraction of time urn  $A$  is empty depends how the balls are initially distributed. Without the additional theory provided in this chapter, one way to determine the fraction of time urn  $A$  is empty would be simulation. The theory in this chapter provides an easy way to determine that fraction.

## 2.9. Chapter Summary

### Key Concepts.

- (1) The states of a Markov chain partition into equivalence classes according to their type: communicating, periodic versus aperiodic, recurrent versus transient, or positive recurrent versus null recurrent.
- (2) Every irreducible, aperiodic Markov chain has a unique nonnegative solution of

$$\begin{aligned}\sum_i \pi_i P_{ij} &= \pi_j \\ \sum_i \pi_i &= 1\end{aligned}$$

called a stationary distribution.

- (3) For an irreducible and aperiodic Markov chain,
  - (a)

$$\lim_{n \rightarrow \infty} (P^n)_{ii} = \frac{1}{m_i} = \pi_{ii}$$

and

- (b)

$$\lim_{n \rightarrow \infty} (P^n)_{ij} = \lim_{n \rightarrow \infty} (P^n)_{ii} = \pi_i.$$

### Vocabulary.

- (1) State  $j$  is **accessible** from state  $i$  if  $(P^n)_{ij} > 0$  for some  $n \geq 1$ .
- (2) The states of a Markov chain partition into equivalence classes according to their type: **communicating**, **periodic** versus **aperiodic**, and **recurrent** versus **transient**, **positive recurrent** versus **null recurrent**.
- (3) The Markov chain is **irreducible** if it has only one communicating class.
- (4) Let the random variable  $\tau_{ii}$  be the **return time** to state  $i$  given the chain starts in  $i$ :

$$\begin{aligned}\tau_{ii} &= \min \{n \geq 1 : X_n = i \mid X_0 = i\}, \\ \tau_{ii} &= \infty \text{ if } X_n \neq i, n \geq 1.\end{aligned}$$

The distribution of  $\tau_{ii}$  is  $f_{ii}^n$ . The **expected return time**  $m_i = \sum_{\nu=1}^{\infty} \nu f_{ii}^{\nu}$ .

- (5) Let the random variable  $\tau_{ij}$  be the **first passage time** to state  $j$  given the chain starts in  $i$ :

$$\begin{aligned}\tau_{ij} &= \min \{n \geq 1 : X_n = j \mid X_0 = i\} \\ \tau_{ij} &= \infty \text{ if } X_n \neq j, n \geq 1.\end{aligned}$$

- (6) If a state  $i$  is recurrent, then it is **positive recurrent** if, starting in  $i$ , the expected time until the process returns to state  $i$  is finite. Otherwise the state is **null recurrent**.
- (7) Positive recurrent and aperiodic states are **ergodic**.

- (8) When the limit exists, let

$$\pi_j = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n \mathbf{1}_{X_\nu=j|X_0=i}$$

denote the **long run proportion of time the chain spends in state  $j$**  or just the *long run proportion* for short.

- (9) For a positive recurrent and aperiodic Markov chain the vector  $(\pi_j)$  satisfies the set of the equations

$$\begin{aligned} \sum_i \pi_i P_{ij} &= \pi_j \\ \sum_i \pi_i &= 1 \end{aligned}$$

and is a **stationary probability distribution** of the Markov chain.

#### Notation.

- (1)  $i, j, l$  – arbitrary or generic state indices
- (2)  $(P^n)_{ij}$  – the  $i, j$  entry of the  $n$ th power of  $P$ .
- (3)  $d(i)$  – the period of a state  $i$
- (4)  $\tau_{ii}$  – the **return time** to state  $i$  given the chain starts in  $i$
- (5)  $\tau_{ij}$  – the time to state  $j$  given the chain starts in  $i$
- (6)  $f_{ii}^n$  – the probability that starting from  $i$ , the first return to state  $i$  occurs at step  $n$
- (7)  $f_i = \mathbb{P}[\tau_{ii} < \infty]$  – the probability that starting in  $i$  the process will *ever* reenter state  $i$
- (8)

$$\pi_j = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n \mathbf{1}_{X_\nu=j|X_0=i}$$

– the **long run proportion of time the chain spends in state  $j$**

- (9)  $m_i$  – the **expected return time**  $\sum_{\nu=1}^{\infty} \nu f_{ii}^\nu$ .

## 2.10. Sources

This section is adapted from: Ross, *Introduction to Probability Models*, Taylor and Karlin, *An Introduction to Stochastic Modeling*, Karlin and Taylor, *A Second Course in Stochastic Processes*. The bathroom example is adapted from the solution in Lessard based on the problem originally posed in The Riddler and Lessard, Lessard. The example of random walk on the non-negative integers is adapted from class notes by Karl Sigman, Sigman.

### 2.11. Algorithms and Scripts

**Data:** State names and transition probability matrix

**Result:** Information about a simple Markov chain

- 1 *Initialization and sample paths*
- 2 Load Markov chain library
- 3 Set state names, set transition probability matrix, set start state
- 4 Set an example length and create a sample path of example length
- 5 *Simulation of stationary distribution and comparison to theoretical*
- 6 Set a long path length, and a transient time
- 7 Create a long sample path
- 8 Slice the long sample path from the transient time to the end
- 9 In the slice count the appearance of each state
- 10 Store in an empirical array
- 11 Compute the theoretical stable array
- 12 **return** *Stable distribution and theoretical stable distribution*

**Algorithm 2:** Markov chain simulation of bathroom example.

R script for Stationary Distributions.

```

1 library("markovchain")
2
3 rows = 6
4
5 stateNames <- c("OCO", "OFO", "OOO", "OOV", "VO", "VV")
6 P <- matrix(c(1/2, 0, 0, 0, 0, 1/2,
7               0, 1/2, 0, 0, 1/4, 1/4,
8               0, 0, 1/2, 0, 1/2, 0,
9               0, 0, 0, 1/2, 1/2, 0,
10              1/6, 1/6, 1/6, 0, 1/2, 0,
11              1/6, 1/6, 0, 1/6, 0, 1/2),
12            nrow=rows, byrow=TRUE)
13 rownames(P) <- stateNames
14 colnames(P) <- stateNames
15
16 startState <- "VV"
17
18 bathroom <- new("markovchain", transitionMatrix=P,
19               states=stateNames, name="Bathroom_
20               Occupancy")
21 print(summary(bathroom))
22
23 pathLength <- 20
24 bathroomHistory <- rmarkovchain(n=pathLength, object=
                bathroom,
                                t0=startState)

```

```

25 cat("A sample history, starting from VV: ",
    bathroomHistory, "\n")
26
27 largeN <- 4000
28 startStable <- 2000
29 history <- rmarkovchain(n=largeN, object=bathroom, t0=
    startState)
30 stablePattern <- history[startStable:largeN]
31 empiricalStable <- c(mean( stablePattern == "OCO" ),
32                     mean( stablePattern == "OFO" ),
33                     mean( stablePattern == "OOO" ),
34                     mean( stablePattern == "OOV" ),
35                     mean( stablePattern == "VO" ),
36                     mean( stablePattern == "VV" )
37                     )
38 theorStable <- steadyStates(bathroom)
39 cat("Empirical stable distribution: ", empiricalStable,
    "\n")
40 cat("Theoretical stable distribution: ", theorStable, "\n
    ")

```

## 2.12. Problems to Work for Understanding

Chapter 2: Classes of States and Stationary Distributions.

2.1: Provide examples of the classifications of states:

- A trivial two-state Markov chain in which neither state is accessible from the other.
- A trivial two-state Markov chain in which both states communicate.
- A Markov chain in which all states have period 2.
- A three-state Markov chain with two states absorbing and one transient state. What states are communicating in this example?
- An irreducible, positive recurrent, and aperiodic three-state Markov chain.

2.2: Randomly distribute three balls between two urns, labeled *A* and *B*. Each period, select an urn at random, and if it is not empty, remove a ball from that urn and put it in the other urn. If the urn is empty, go to the next period. Make a Markov chain model of this situation and classify all states. In the long run what fraction of time is urn *A* empty? Does this depend on how the balls are initially distributed between the two urns?

2.3: A professor has  $n$  umbrellas, of which initially  $k \in (0, n)$  are at home and  $n - k$  are at work. Every day, the professor walks to work in the morning and returns home in the evening. In each trip, the professor takes an umbrella only if it is raining. Assume that in every trip between home and work or back, the chance of rain is  $p = 1/2$ , independently of other trips.

- Model this process as a Markov chain.
- Determine the stationary distribution.



(3) Asymptotically, in what fraction of trips does the professor get wet?

This is a standard problem appearing in many texts on Markov chains in various degrees of generality.

2.4: Assume the fraction of oblivious, forgetful, and conscientious users are  $p$ ,  $q$ , and  $r$  respectively, with  $0 \leq p, q, r \leq 1$  and  $p + q + r = 1$ . Solve the bathroom problem under this general assumption.

2.5: Assume the fraction of oblivious, forgetful, and conscientious users are  $p$ ,  $q$ , and  $r$  respectively, with  $0 \leq p, q, r \leq 1$  and  $p + q + r = 1$ . Further assume the bathroom is occupied  $2/3$  of the time, and vacant  $1/3$  of the time. Solve the bathroom problem under this general assumption.

2.6: Assume the fraction of oblivious, forgetful, and conscientious users are  $p$ ,  $q$ , and  $r$  respectively, with  $0 \leq p, q, r \leq 1$  and  $p + q + r = 1$ . Further assume the bathroom is occupied  $1 - v$  of the time, and vacant  $v$  of the time, where  $0 < v < 1$ . Solve the bathroom problem under this general assumption. What happens as  $v \rightarrow 0$  or  $v \rightarrow 1$ ?

2.7: Assume the fraction of oblivious, forgetful, and conscientious users are  $p$ ,  $q$ , and  $r$  respectively, with  $0 \leq p, q, r \leq 1$  and  $p + q + r = 1$ . Also assume that the oblivious people spend twice as long in the bathroom as the conscientious or forgetful people. Assume the bathroom is vacant  $v$  of the time, where  $0 < v < 1$ . Find the transition probability matrix. What is the condition on  $v$  to make the probabilities consistent?

2.8: Prove Corollary 2.22:

- (1) For any communication class  $C$  of a Markov chain, all states in  $C$  are either recurrent or all states in  $C$  are transient. That is
  - if  $i$  and  $j$  communicate, and  $i$  is recurrent, then so is  $j$
  - if  $i$  and  $j$  communicate, and  $i$  is transient, then so is  $j$ .
- (2) For an irreducible Markov chain, either all states are recurrent or all states are transient.

2.9: Prove  $f_{ij}^n = \sum_{\nu=0}^n f_{ij}^{\nu} P_{jj}^{\nu-k}$ .

2.10: If  $a_n \rightarrow a$  as  $n \rightarrow \infty$ , then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n a_{\nu} = a,$$

so that if  $a_n$  converges to  $a$ , the sequence of averages converges to  $a$ .

2.11: Using the notation in the proof of Lemma 2.31, suppose that the bounded sequence  $u_n$  satisfies the renewal equation

$$u_n - \sum_{k=0}^n a_k u_{n-k} = b_n$$

where  $a_k \geq 0$  for all  $n$ ,  $a_1 > 0$ ,  $\sum_{k=0}^{\infty} a_k = 1$  and  $b_k \geq 0$ . Let  $\mu = \liminf_{n \rightarrow \infty} u_n$  with a subsequence such that  $\lim_{j \rightarrow \infty} u_{n_j} = \mu$ , then  $\lim_{j \rightarrow \infty} u_{n_j-d} = \mu$  for each integer  $d$ .

---

2.12: For the random walk restricted to the nonnegative integers with  $P_{0,1} = 1$  and otherwise,  $P_{i,i-1} = p$  with  $p > 1/2$  and  $P_{i,i+1} = 1 - p < 1/2$ , show that the stationary distribution is  $\pi_0 = \frac{2p-1}{2p}$  and  $\pi_\nu = \frac{2p-1}{2p} \left( \frac{(1-p)^{\nu-1}}{p^\nu} \right)$  for  $\nu \geq 1$ .



## Waiting Time to Absorption

Let  $\{X_n\}$  be a finite-state absorbing Markov chain with  $a$  absorbing states and  $t$  transient states, where  $a + t = k$ . Starting at one of the transient states  $i$  where  $a + 1 \leq i \leq a + t$  such a process will remain in the transient states for some duration. Ultimately, the process gets trapped in one of the absorbing states  $i = 1, \dots, a$ . Before the Markov chain transitions to one of the absorbing states, the number of times it visits a transient state is a random variable. Let  $Y_{ij}$  denote the number of visits the system makes to transient state  $j$  before reaching an absorbing state, given the system started in transient state  $i$ . Thus,  $Y_{ij}$  is a discrete random variable that can take on any nonnegative integer value. The random variables  $Y_{ij}$  are the fundamental random variables of interest here. These fundamental random variables are the building blocks for constructing and investigating other random variables. The mean, variance and covariances of the  $Y_{ij}$  are the first statistics to investigate. Of special interest is the mean time until absorption.

Mathematically Mature: contains mathematics beyond calculus with proofs.

### 3.1. Chapter Starter Question

For a Markov chain with an absorbing state, describe the random variable for the time until the chain gets absorbed.

### 3.2. Theory

Let  $\{X_n\}$  be a finite-state absorbing Markov chain with  $a$  absorbing states and  $t$  transient states, where  $a + t = k$ . Let the  $(a + t) \times (a + t)$  transition probability matrix be  $P$ . Order the states so the absorbing states come first and non-absorbing, i.e. transient, states come last. The states  $a + 1, a + 2, \dots, a + t$  are transient in that  $(P^n)_{ij} \rightarrow 0$  as  $n \rightarrow \infty$  for  $a + 1 \leq i, j \leq a + t$ , while states  $1, \dots, a$  are absorbing,  $P_{ii} = 1$  for  $1 \leq i \leq a$ . Then the transition probability matrix has the block-matrix

form

$$P = \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix}.$$

Here  $I_a$  is an  $a \times a$  identity matrix,  $A$  is the  $t \times a$  matrix of single-step transition probabilities from the  $t$  transient states to the  $a$  absorbing states,  $T$  is a  $t \times t$  submatrix of single-step transition probabilities among the transient states, and  $0$  is a  $a \times t$  matrix of 0s representing the single-step transition probabilities from absorbing states to transient states.

Starting at one of the transient states  $i$  where  $a + 1 \leq i \leq a + t$  such a process will remain in the transient states for some duration. Ultimately, the process gets trapped in one of the absorbing states  $i = 1, \dots, a$ . Before the Markov chain transitions to one of the absorbing states, the number of times it visits a transient state is a random variable. Let  $Y_{ij}$  denote the number of visits the system makes to transient state  $j$  before reaching an absorbing state, given the system started in transient state  $i$ . Thus,  $Y_{ij}$  is a discrete random variable that can take on any nonnegative integer value. The random variables  $Y_{ij}$  are the fundamental random variables of interest here. These fundamental random variables are the building blocks for constructing and investigating other random variables. The mean, variance and covariances of the  $Y_{ij}$  are the first statistics to investigate. Of special interest is the mean time until absorption. Define the **absorption time**

$$w_i = \min \{n \geq 0 : X_n \leq a \mid X_0 = i\}.$$

Notice  $w_i = \sum_{j=a+1}^{a+t} Y_{ij}$ , the total number of visits the process makes among the transient states. The expected value of this random time,  $\mathbb{E}[w_i]$  for  $i = a+1, \dots, a+t$ , is a first measure of the random variable  $w_i$ . Also of interest is the probability distribution of the states into which absorption takes place. Using the fundamental random variables, it is possible to compute this probability too.

### 3.3. Indicator Bernoulli Random Variables

Let the indicator random variables be

$$\mathbf{1}_{ij}^{(m)} = \begin{cases} 1 & \text{if the Markov chain is in transient state } j \\ & \text{after } m \text{ steps given that it starts in transient state } i \\ 0 & \text{if the Markov chain is not in transient state } j \\ & \text{after } m \text{ steps given that it starts in transient state } i \end{cases}$$

for  $m = 0, 1, 2, \dots$ . The case  $m = 0$  simply indicates where the system starts, with the usual notation,  $\mathbf{1}_{ij}^{(0)}$  is the Kronecker delta function,  $\delta_{ij}$ . The indicator random variables connect to the fundamental random variables  $Y_{ij}$  through the sum

$$Y_{ij} = \sum_{m=0}^{\infty} \mathbf{1}_{ij}^{(m)}.$$

### 3.4. Expected Number of Visits Between States

The expected number of visits to transient state  $j$  given the Markov chain starts in transient state  $i$  in terms of the indicator random variable is

$$\mathbb{E}[Y_{ij}] = \mathbb{E} \left[ \sum_{m=0}^{\infty} \mathbf{1}_{ij}^{(m)} \right] = \sum_{m=0}^{\infty} \mathbb{E} \left[ \mathbf{1}_{ij}^{(m)} \right].$$

Use mathematical induction to show

$$P^m = \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix}^{m-1} \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix} = \begin{pmatrix} I_a & 0 \\ (I_t + T + T^2 + \cdots + T^{m-1})A & T^m \end{pmatrix}.$$

(See the exercises.) The elements  $(P^m)_{ij}$  of  $P^m$  are the  $m$ -step transition probabilities between all states. Since  $\mathbb{E}[\mathbf{1}_{ij}^{(m)}] = (P^m)_{ij}$ , so

$$\mathbb{E}[Y_{ij}] = \sum_{m=0}^{\infty} \mathbb{E}[\mathbf{1}_{ij}^{(m)}] = \sum_{m=0}^{\infty} (P^m)_{ij}.$$

When  $i$  and  $j$  are transient states, consider the entries in the transient corner matrix  $T^m$ , so

$$\mathbb{E}[Y_{ij}] = \sum_{m=0}^{\infty} (T^m)_{ij} = \left( \sum_{m=0}^{\infty} T^m \right)_{ij}.$$

The basic theory of finite absorbing Markov chains ensures that the induced 2-norm (or operator norm) of  $T$  is less than 1 under typical conditions, that is  $\|T\| < 1$ . (See the exercises.) Therefore  $\sum_{m=0}^{\infty} T^m$  converges. Furthermore, it converges to the **fundamental matrix**  $N = (I - T)^{-1}$ . (See the exercises.) Thus  $\mathbb{E}[Y_{ij}] = N_{ij}$ .

### 3.5. Waiting Time to Absorption

**Theorem 3.1.** *The entries  $N_{ij}$  of the fundamental matrix are the expected number of times the chain started from state  $i$  will be in state  $j$  before ultimate absorption and the vector of expected waiting times to absorption is  $\mathbb{E}[\mathbf{w}] = N = (I - T)^{-1}\mathbf{1}$ .*

**Proof.** The sum over all states  $j$  of the expected number of times that the chain started from state  $i$  will be in state  $j$  before ultimate absorption is the expected waiting time to absorption.  $\square$

### 3.6. Covariances of Numbers of Visits Between States

Now use the indicator Bernoulli random variables to derive  $\text{Cov}[Y_{ij}, Y_{il}]$  where  $i, j, l$  are transient states. Recall

$$\text{Cov}[Y_{ij}, Y_{il}] = \mathbb{E}[Y_{ij} \cdot Y_{il}] - \mathbb{E}[Y_{ij}] \cdot \mathbb{E}[Y_{il}]$$

and since  $\mathbb{E}[Y_{ij}]$  and  $\mathbb{E}[Y_{il}]$  are known, all that is necessary is  $\mathbb{E}[Y_{ij} \cdot Y_{il}]$ . Start with

$$Y_{ij}Y_{il} = \left( \sum_{\nu=0}^{\infty} \mathbf{1}_{ij}^{(\nu)} \right) \left( \sum_{\mu=0}^{\infty} \mathbf{1}_{il}^{(\mu)} \right) = \sum_{\nu=0}^{\infty} \sum_{\mu=0}^{\infty} \mathbf{1}_{ij}^{(\nu)} \mathbf{1}_{il}^{(\mu)}$$

so

$$\mathbb{E}[Y_{ij}Y_{il}] = \mathbb{E}\left[\sum_{\nu=0}^{\infty}\sum_{\mu=0}^{\infty}\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\mu)}\right] = \sum_{\nu=0}^{\infty}\sum_{\mu=0}^{\infty}\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\mu)}\right].$$

Rearrange the double sum into 3 double sums, summing first in  $\mu$  over the lattice points above the line  $\mu = \nu$ , a second term summing over the lattice points along the line  $\mu = \nu$ , and last summing first in  $\nu$  over lattice points below the line  $\mu = \nu$ ,

$$\sum_{\nu=0}^{\infty}\sum_{\mu=\nu+1}^{\infty}\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\mu)}\right] + \sum_{\nu=0}^{\infty}\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\nu)}\right] + \sum_{\mu=0}^{\infty}\sum_{\nu=\mu+1}^{\infty}\mathbb{E}\left[\mathbf{1}_{il}^{(\mu)}\mathbf{1}_{ij}^{(\nu)}\right].$$

The first and third terms are symmetric, so only evaluate the first term.

The expression  $\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\mu)}\right]$  is the probability that the system is in transient state  $j$  after exactly  $\nu$  steps from the start in state  $i$  and the system is in transient state  $l$  after exactly  $\mu$  steps from the start in state  $i$ . In the first double sum  $\nu < \mu$ . Using the Markov chain property, this is  $\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\mu)}\right] = p_{ij}^{(\nu)}p_{jl}^{(\mu-\nu)}$ . Therefore, the first term is

$$\begin{aligned} \sum_{\nu=0}^{\infty}\sum_{\mu=\nu+1}^{\infty}\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\mu)}\right] &= \sum_{\nu=0}^{\infty}\sum_{\mu=\nu+1}^{\infty}p_{ij}^{(\nu)}p_{jl}^{(\mu-\nu)} = \sum_{\nu=0}^{\infty}\sum_{\mu=\nu+1}^{\infty}p_{ij}^{(\nu)}p_{jl}^{(\mu-\nu)} \\ &= \sum_{\nu=0}^{\infty}\sum_{z=1}^{\infty}p_{ij}^{(\nu)}p_{jl}^{(z)} = \left(\sum_{\nu=0}^{\infty}p_{ij}^{(\nu)}\right)\left(\sum_{z=1}^{\infty}p_{jl}^{(z)}\right) = \left(\sum_{\nu=0}^{\infty}p_{ij}^{(\nu)}\right)\left(\sum_{z=0}^{\infty}p_{jl}^{(z)} - p_{jl}^{(0)}\right) \\ &= \left(\sum_{\nu=0}^{\infty}(T^{\nu})_{ij}\right)\left(\sum_{z=0}^{\infty}(T^z)_{jl} - \delta_{jl}\right) = \left(\sum_{\nu=0}^{\infty}T^{\nu}\right)_{ij}\left(\sum_{z=0}^{\infty}T^z - \delta_{jl}\right)_{jl} \\ &= ((I_t - T)^{-1})_{ij}((I_t - T)^{-1} - \delta_{jl})_{jl} = N_{ij}(N_{jl} - \delta_{jl}). \end{aligned}$$

The third double sum is the first double sum with  $j$  and  $l$  interchanged, so

$$\sum_{\mu=0}^{\infty}\sum_{\nu=\mu+1}^{\infty}\mathbb{E}\left[\mathbf{1}_{il}^{(\mu)}\mathbf{1}_{ij}^{(\nu)}\right] = N_{il}(N_{lj} - \delta_{lj}).$$

Finally, the second term is  $\sum_{\nu=0}^{\infty}\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\nu)}\right]$  where each summand is the probability the Markov chain is in transient state  $j$  after exactly  $\nu$  steps after starting in transient state  $i$  and simultaneously in state  $l$  after exactly  $\nu$  steps starting from transient state  $i$ . This is only possible if  $j = l$  hence  $\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\nu)}\right] = p_{ij}^{(\nu)}\delta_{jl}$ . Thus for the second term

$$\sum_{\nu=0}^{\infty}\mathbb{E}\left[\mathbf{1}_{ij}^{(\nu)}\mathbf{1}_{il}^{(\nu)}\right] = \sum_{\nu=0}^{\infty}p_{ij}^{(\nu)}\delta_{jl} = \left(\sum_{\nu=0}^{\infty}(T^{\nu})_{ij}\right)\delta_{jl} = \left(\sum_{\nu=0}^{\infty}T^{\nu}\right)_{ij}\delta_{jl} = N_{ij}\delta_{jl}.$$

Putting all terms together

$$\mathbb{E}[Y_{ij}Y_{il}] = N_{ij}(N_{jl} - \delta_{jl}) + N_{ij}\delta_{jl} + N_{il}(N_{lj} - \delta_{lj}) = N_{ij}N_{jl} + N_{il}N_{lj} - N_{il}\delta_{lj}.$$

Then

$$\begin{aligned} \text{Cov}[Y_{ij}, Y_{il}] &= \mathbb{E}[Y_{ij}Y_{il}] - \mathbb{E}[Y_{ij}]\mathbb{E}[Y_{il}] \\ (3.1) \quad &= N_{ij}N_{jl} + N_{il}N_{lj} - N_{ij}N_{il} - N_{il}\delta_{lj}. \end{aligned}$$

The result is symmetric under the interchange of  $j$  and  $l$  as it should be.

In particular, letting  $j = l$  gives the variance of the number of visits to state  $j$  starting from  $i$ :

$$\text{Var}[Y_{ij}] = 2N_{ij}N_{jj} - N_{ij}^2 - N_{ij}.$$

Define  $\text{diag}(N)$  to be the diagonal matrix setting all off-diagonal elements of  $N$  to 0, and define  $N_{\text{sq}}$  to be the matrix resulting from squaring each entry, then

$$\text{Var}[Y_{(i)}] = N(2\text{diag}(N) - I) - N_{\text{sq}}.$$

Note that this is the variance of the number of visits to transient state  $j$  when starting from transient state  $i$ , *not* the variance of the waiting time to an absorbing state. The variance of the waiting time until absorption into any state from state  $i$  is the sum of all  $t^2$  entries in  $\text{Var}[Y_{(i)}]$ .

The covariance, for a fixed  $i$ , is the  $t \times t$  matrix of entries  $\text{Cov}[Y_{ij}, Y_{il}]$ . Letting  $N_{(i,\cdot)}$  denote the  $1 \times t$  row-vector from row  $i$  and setting  $(\text{diag } N_{(i,\cdot)})$  to be the diagonal matrix with this vector along the diagonal this becomes

$$[\text{Cov}[Y_{ij}, Y_{il}]] = (\text{diag } N_{(i,\cdot)})N + N^T(\text{diag } N_{(i,\cdot)}) - N_{(i,\cdot)}^T N_{(i,\cdot)} - \text{diag } N_{(i,\cdot)}.$$

Note the outer product  $N_{(i,\cdot)}^T N_{(i,\cdot)}$ . Note also the notation  $[\text{Cov}[Y_{ij}, Y_{il}]]$  for the matrix with  $j, l$  entry  $\text{Cov}[Y_{ij}, Y_{il}]$ .

### 3.7. First-Step Analysis

First-step analysis says the absorption time from state  $i$  is the first step to another transient state plus a weighted average, according to the transition probabilities over the transient states, of the absorption times from the other transient states. In symbols, first-step analysis says

$$w_i = 1 + \sum_{j=a+1}^{a+t} P_{ij}w_j.$$

As before, for a Markov chain with  $a$  absorbing states and  $t$  transient states, re-order the states so the absorbing states come first and non-absorbing, i.e. transient, states come last. Then the transition matrix has the canonical form:

$$P = \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix}.$$

Here  $I_a$  is an  $a \times a$  identity matrix,  $A$  is the  $t \times a$  matrix of single-step transition probabilities from the  $t$  transient states to the  $a$  absorbing states,  $T$  is a  $t \times t$  submatrix of single-step transition probabilities among the transient states, and  $0$  is a  $a \times t$  matrix of 0s representing the single-step transition probabilities from absorbing states to transient states.

Expressing the first-step analysis compactly in vector-matrix form as

$$\mathbf{w} = \mathbf{1} + T\mathbf{w}$$

or

$$(I - T)\mathbf{w} = \mathbf{1}.$$

Then  $\mathbf{w} = (I - T)^{-1}\mathbf{1}$ . The matrix  $N = (I - T)^{-1}$  is the **fundamental matrix** for the absorbing Markov chain. The entries  $N_{ij}$  of this matrix have a probabilistic



interpretation. The entries  $N_{ij}$  are the expected number of times the chain started from state  $i$  will be in state  $j$  before ultimate absorption.

The next theorem shows the  $t \times a$  matrix of **absorption probabilities**  $B = NA = (I - T)^{-1}A$  has as entries the probability of starting at state  $i$  and ending up at a given absorbing state  $j$ .

**Theorem 3.2.** *Let  $b_{ij}$  be the probability of the Markov chain starting in transient state  $i$  and ending in absorbing state  $j$ , then*

$$B = (b_{ij}) = NA.$$

**Proof.** The proof is by first-step analysis. Starting in state  $i$ , the process may be captured in  $j$  in one or more steps. The probability of capture in a single step is  $p_{ij}$ . If this does not happen, the process may move to another absorbing state, in which case it is impossible to reach  $j$ , or to a transient state  $k$ . In the latter case, the probability of being captured in  $j$  is  $b_{kj}$ . Hence

$$b_{ij} = p_{ij} + \sum_{l=a+1}^{a+t} p_{il}b_{lj}$$

or in matrix form  $B = A + TB$ . Thus,  $B = (I - T)^{-1}A = NA$ .  $\square$

Kemeny and Snell [KS60, page 51] derive the variance of the waiting time using first-step analysis.

**Theorem 3.3.**

$$\text{Var}[\mathbf{w}] = (2N - I)N\mathbf{1} - (N\mathbf{1})_{sq}$$

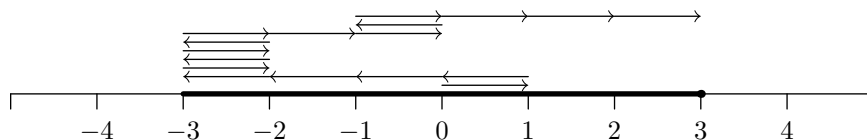
where  $(N\mathbf{1})_{sq}$  is the element-wise squared vector.

**Proof.** (1) Start with  $\mathbb{E}[\mathbf{w}] = N\mathbf{1}$ . Let  $\mathbf{w}_{sq}$  be the element-wise squared vector. Then use first-step analysis to evaluate  $\mathbb{E}[\mathbf{w}_{sq}]$ .

(2) From starting state  $i$  the chain can go to any state  $l$  with probability  $p_{il}$ . If the new state is absorbing, then it can never reach another state, and the contribution is 1 step. If the new state is transient count the weighted average of the squares of the waiting times plus 1.

(3) In symbols:

$$\begin{aligned} \mathbb{E}[\mathbf{w}_{sq}] &= \sum_{l=1}^a p_{il}\mathbf{1} + \sum_{l=a+1}^{a+t} p_{il}(\mathbb{E}[(\mathbf{w} + \mathbf{1})_{sq}])_l \\ &= \sum_{l=1}^a p_{il}\mathbf{1} + \sum_{l=a+1}^{a+t} p_{il} \left( (\mathbb{E}[\mathbf{w}_{sq}])_l + 2(\mathbb{E}[\mathbf{w}])_l + \mathbf{1} \right) \\ &= T\mathbb{E}[\mathbf{w}_{sq}] + 2T\mathbb{E}[\mathbf{w}] + \mathbf{1}. \end{aligned}$$



(4) Rearrange using  $N = (I_t - T)^{-1}$  and  $NT = (I_t - T)^{-1}T = N - I_t$  (See the exercises.)

$$\begin{aligned}\mathbb{E}[\mathbf{w}_{sq}] &= (I_t - T)^{-1}(2T\mathbb{E}[\mathbf{w}] + \mathbf{1}) \\ &= 2NTE[\mathbf{w}] + N\mathbf{1} \\ &= 2(N - I_t)\mathbb{E}[\mathbf{w}] + \mathbb{E}[\mathbf{w}] \\ &= (2N - I_t)\mathbb{E}[\mathbf{w}].\end{aligned}$$

(5) Thus

$$\text{Var}[\mathbf{w}] = (2N - I)N\mathbf{1} - (N\mathbf{1})_{\text{sq}}.$$

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**Remark 3.4.** Carchidi and Higgins [CH17] give an alternate proof and slightly different derivation of this formula for the variance of the waiting time until absorption using equation (3.1).

### 3.8. Examples

**Example 3.5.** Consider a random walk of a particle that moves along a straight line in unit steps. Each step is 1 unit to the right with probability  $p$  and to the left with probability  $q = 1 - p$ . It moves until it reaches one of two extreme points which are absorbing boundaries. Assume that if the process reaches the boundary points, it remains there from that time on. Figure 3.1 has 9 states numbered from  $-4$  to  $4$ . The absorbing boundary states are  $-4$  and  $4$ .

The full transition probability matrix is

[illegible]

Reorder the states as  $-4, 4, -3, -2, -1, 0, 1, 2, 3$  to bring the transition probability matrix to the standard form

$$P_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ q & 0 & 0 & p & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q & 0 & p & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & q & 0 & p & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & q & 0 & p & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & q & 0 & p & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & q & 0 & p \\ 0 & p & 0 & 0 & 0 & 0 & 0 & q & 0 \end{pmatrix}$$

so

$$T = \begin{pmatrix} 0 & p & 0 & 0 & 0 & 0 & 0 \\ q & 0 & p & 0 & 0 & 0 & 0 \\ 0 & q & 0 & p & 0 & 0 & 0 \\ 0 & 0 & q & 0 & p & 0 & 0 \\ 0 & 0 & 0 & q & 0 & p & 0 \\ 0 & 0 & 0 & 0 & q & 0 & p \\ 0 & 0 & 0 & 0 & 0 & q & 0 \end{pmatrix}.$$

A computer algebra system can compute the fundamental matrix  $N(p) = (I - T)^{-1}$  but the general form in  $p$  and  $q$  is long and unhelpful. Two representative numerical examples suffice to show the possibilities.

$$N(1/2) = \begin{pmatrix} 7/4 & 3/2 & 5/4 & 1 & 3/4 & 1/2 & 1/4 \\ 3/2 & 3 & 5/2 & 2 & 3/2 & 1 & 1/2 \\ 5/4 & 5/2 & 15/4 & 3 & 9/4 & 3/2 & 3/4 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 \\ 3/4 & 3/2 & 9/4 & 3 & 15/4 & 5/2 & 5/4 \\ 1/2 & 1 & 3/2 & 2 & 5/2 & 3 & 3/2 \\ 1/4 & 1/2 & 3/4 & 1 & 5/4 & 3/2 & 7/4 \end{pmatrix}.$$

Then the waiting times to absorption are 7, 12, 15, 16, 15, 12, 7. For the variances, consider only the central state, originally labeled as 0, after reordering it is the sixth state in the middle of the transient states.

$$[\text{Cov } [Y_{0j}, Y_{0l}]] = \begin{pmatrix} 3/2 & 5/2 & 2 & 1 & 0 & -1/2 & -1/2 \\ 5/2 & 6 & 13/2 & 4 & 3/2 & 0 & -1/2 \\ 2 & 13/2 & 21/2 & 9 & 9/2 & 3/2 & 0 \\ 1 & 4 & 9 & 12 & 9 & 4 & 1 \\ 0 & 3/2 & 9/2 & 9 & 21/2 & 13/2 & 2 \\ -1/2 & 0 & 3/2 & 4 & 13/2 & 6 & 5/2 \\ -1/2 & -1/2 & 0 & 1 & 2 & 5/2 & 3/2 \end{pmatrix}.$$

The variance of the number of visits to 0 until absorption is  $\mathbf{1}^T V \mathbf{1} = 160$ , the standard deviation is  $4\sqrt{10}$ . The negative covariance  $-1/2$  of the number of visits from 0 to  $-3$  until absorption with the number of visits from 0 to 3 until absorption indicates the random number of visits from 0 to  $-3$  until absorption has a somewhat opposite distribution to that of the random number of visits from 0 to 3 until absorption. That is, when the number of visits from 0 to  $-3$  until absorption is

large, the number of visits from 0 to 3 until absorption will be small. This makes sense, since if the number of visits from 0 to  $-3$  is large, the likelihood of absorption into  $-4$  increases, and the number of visits from 0 to 3 decreases.

The probabilities of absorption are

$$N(1/2)A = \begin{pmatrix} 7/8 & 1/8 \\ 3/4 & 1/4 \\ 5/8 & 3/8 \\ 1/2 & 1/2 \\ 3/8 & 5/8 \\ 1/4 & 3/4 \\ 1/8 & 7/8 \end{pmatrix}$$

and are symmetric as expected.

If  $p = 2/3$  so the probability of moving to the right is twice the probability of moving to the left, then

$$N(2/3) = \begin{pmatrix} 127/85 & 126/85 & 124/85 & 24/17 & 112/85 & 96/85 & 64/85 \\ 63/85 & 189/85 & 186/85 & 36/17 & 168/85 & 144/85 & 96/85 \\ 31/85 & 93/85 & 217/85 & 42/17 & 196/85 & 168/85 & 112/85 \\ 3/17 & 9/17 & 21/17 & 45/17 & 42/17 & 36/17 & 24/17 \\ 7/85 & 21/85 & 49/85 & 21/17 & 217/85 & 186/85 & 124/85 \\ 3/85 & 9/85 & 21/85 & 9/17 & 93/85 & 189/85 & 126/85 \\ 1/85 & 3/85 & 7/85 & 3/17 & 31/85 & 63/85 & 127/85 \end{pmatrix}$$

and the waiting times to absorption are approximately 9.05, 12.07, 12.08, 10.59, 8.34, 5.72, 2.91. For the variances, consider only the central state, originally labeled as 0 and after reordering is the sixth state in the middle of the transient states.

$$[\text{Cov}[Y_{0j}, Y_{0k}]] = \begin{pmatrix} \frac{462}{1445} & \frac{162}{289} & \frac{708}{1445} & \frac{72}{289} & 0 & -\frac{144}{1445} & -\frac{144}{1445} \\ \frac{162}{289} & \frac{2232}{1445} & \frac{2682}{1445} & \frac{324}{289} & \frac{504}{1445} & 0 & -\frac{144}{1445} \\ \frac{708}{1445} & \frac{2682}{1445} & \frac{5124}{1445} & \frac{882}{289} & \frac{1764}{1445} & \frac{504}{1445} & 0 \\ \frac{72}{289} & \frac{324}{289} & \frac{882}{289} & \frac{1260}{289} & \frac{882}{289} & \frac{324}{289} & \frac{72}{289} \\ 0 & \frac{504}{1445} & \frac{1764}{1445} & \frac{882}{289} & \frac{5838}{1445} & \frac{720}{289} & \frac{912}{1445} \\ -\frac{144}{1445} & 0 & \frac{504}{1445} & \frac{324}{289} & \frac{720}{289} & \frac{4068}{1445} & \frac{1728}{1445} \\ -\frac{144}{1445} & -\frac{144}{1445} & 0 & \frac{72}{289} & \frac{912}{1445} & \frac{1728}{1445} & \frac{1176}{1445} \end{pmatrix}.$$

The variance is  $\mathbf{1}^T V \mathbf{1} = 15264/289 \approx 52.817$ , the standard deviation is 7.268, less than the symmetric case where  $p = 1/2 = q$ , as expected.

The probabilities of absorption are

$$N(2/3)A = \begin{pmatrix} 127/255 & 128/255 \\ 21/85 & 64/85 \\ 31/255 & 224/255 \\ 1/17 & 16/17 \\ 7/255 & 248/255 \\ 1/85 & 84/85 \\ 1/255 & 254/255 \end{pmatrix}.$$

The absorption probabilities are strongly biased to the right, as expected.  $\nabla$

**Example 3.6.** An urn contains two unpainted balls. At a sequence of times, choose a ball at random, then paint it either red or black, and put it back. For an unpainted ball, choose a color at random. For a painted ball, change its color. Form a Markov chain by taking as a state the triple  $(x, y, z)$  where  $x$  is the number of unpainted balls,  $y$  the number of red balls, and  $z$  the number of black balls. The transition matrix is then

$$\begin{array}{c} (0, 1, 1) \quad (0, 2, 0) \quad (0, 0, 2) \quad (2, 0, 0) \quad (1, 1, 0) \quad (1, 0, 1) \\ \begin{pmatrix} (0, 1, 1) & 0 & 1/2 & 1/2 & 0 & 0 & 0 \\ (0, 2, 0) & 1 & 0 & 0 & 0 & 0 & 0 \\ (0, 0, 2) & 1 & 0 & 0 & 0 & 0 & 0 \\ (2, 0, 0) & 0 & 0 & 0 & 0 & 1/2 & 1/2 \\ (1, 1, 0) & 1/4 & 1/4 & 0 & 0 & 0 & 1/2 \\ (1, 0, 1) & 1/4 & 0 & 1/4 & 0 & 1/2 & 0 \end{pmatrix} \end{array}.$$

In this case, the system has no absorbing state, that is, a state that once entered remains the same thereafter. However, the first three states together are an irreducible set, once the process enters that set, it continues in that set. So lump those states together as a single absorbing state, and the transient states are  $(2, 0, 0)$ ,  $(1, 1, 0)$ , and  $(1, 0, 1)$ . Then

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

and the fundamental matrix is

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

With this,

$$\mathbb{E}[\mathbf{w}] = N\mathbf{1} = (3, 2, 2)^T$$

and

$$\text{Var}[\mathbf{w}] = (2N - I)\mathbb{E}[\mathbf{w}] - (\mathbb{E}[\mathbf{w}])_{\text{sq}} = (2, 2, 2)^T.$$

Finally,

$$\text{Var}[\mathbf{X}] = N(2 \text{diag}(N) - I) - N_{\text{sq}} = \begin{pmatrix} 0 & 2/3 & 2/3 \\ 0 & 4/9 & 2/3 \\ 0 & 2/3 & 4/9 \end{pmatrix}.$$

Since the process must immediately leave state  $(2, 0, 0)$  and cannot go back, the variance is 0 for the number of times in this state.  $\nabla$

**Example 3.7.** The following is a larger example of the painting the balls puzzle.

You play a game with four balls in a box: One ball is red, one is blue, one is green and one is yellow. You draw a ball out of the box at random and note its color. Without replacing the first ball, you draw a second ball and then paint it to match the color of the first. Replace both balls, and repeat the process. The game ends when all four balls have become the same color. What is the expected number of turns to finish the game?

Take the states as the number of balls of each different color without regard for the colors themselves. For example, partition 4 balls in 5 different ways:

$$1 + 1 + 1 + 1, \quad 2 + 1 + 1, \quad 2 + 2, \quad 3 + 1, \quad 4.$$

The partition  $2 + 1 + 1$ , for example, consists of cases where two of the balls are the same color and the other two balls are two other colors. For example, the cases “red & red & green & blue” and “blue & blue & yellow & red” correspond to the partition  $2 + 1 + 1$ . Using these five partitions as states in a Markov Chain, compute the transition probabilities to go from one state to the next. For example, the probability of transition from  $2 + 1 + 1$  to  $3 + 1$  is  $1/3$  because in order for this transition to occur, first choose one of the two identically colored balls with probability  $2/4$ , then choose one of the other two balls out of the remaining three with probability  $2/3$ . The joint probability is  $2/4 \cdot 2/3 = 1/3$ . As another example, the probability of transition from  $2 + 2$  to  $3 + 1$  is the probability of first picking a ball of either color, leaving 1 ball of that color and 2 balls of the other color, then from those 3 balls picking the second color with probability  $2/3$ . Calculate all remaining transition probabilities in the same way.

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

The absorbing state is 4. Rearranging into the canonical block-matrix form

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

Then  $N = (I - T)^{-1}$  is

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

and the waiting time from the initial state is  $1 + 2 + 4 + 2 = 9$ . From the state  $1 + 1 + 1 + 1$  (labeled as state 2 in the canonical format), the covariance matrix is

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 12 & 6 \\ 0 & 0 & 6 & 6 \end{pmatrix}.$$

Then the variance of the number of visits is 32 and the standard deviation of the number of visits is  $4\sqrt{2} \approx 5.657$ .

▽

**Example 3.8.** It's your 30th birthday, and your friends bought you a cake with 30 candles on it. You make a wish and try to blow them out. Every time you blow, you blow out a random number of candles between one and the number that remain, including one and that other number. How many times on average do you blow before you extinguish all the candles?

Let the states be the number of candles remaining lit. Order the  $N = 31$  states as  $0, 1, 2, 3, \dots, 29, 30$ . Then the state 0 is absorbing and all other states are transient. Interpret “blow out a random number of candles between one and the number that remain” as uniform distribution on the number of candles remaining. Instead of solving this full problem at once, try a smaller problem first, with the number of candles  $N = 5$ . Then the transition probability matrix in canonical form is

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 & 0 \\ 1/3 & 1/3 & 1/3 & 0 & 0 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 & 0 & 0 \\ 1/5 & 1/5 & 1/5 & 1/5 & 1/5 & 0 \end{pmatrix}.$$

Then the first-step equations for the waiting time, that is the number of attempts needed to blow out the candles are

$$\begin{aligned} w_1 &= 1 \\ w_2 &= 1 + \frac{1}{2}w_1 \\ w_3 &= 1 + \frac{1}{3}w_1 + \frac{1}{3}w_2 \\ w_4 &= 1 + \frac{1}{4}w_1 + \frac{1}{4}w_2 + \frac{1}{4}w_3 \\ w_5 &= 1 + \frac{1}{5}w_1 + \frac{1}{5}w_2 + \frac{1}{5}w_3 + \frac{1}{5}w_4 \end{aligned}$$

Solving this recursively,  $w_1 = 1$ ,  $w_2 = 1 + \frac{1}{2}$ ,  $w_3 = 1 + \frac{1}{3} + \frac{1}{3} \cdot (1 + \frac{1}{2})$ , so  $w_3 = 1 + \frac{1}{2} + \frac{1}{3}$ . Continuing to solve recursively

$$\begin{aligned} w_4 &= 1 + 1/2 + 1/3 + 1/4 \\ w_5 &= 1 + 1/2 + 1/3 + 1/4 + 1/5. \end{aligned}$$

The inductive pattern is clear. The waiting time with  $N$  candles is the  $N$ th **harmonic number**  $H_N$

$$w_N = H_N = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \dots + \frac{1}{N}.$$

For the original problem with 30 candles the transient states are  $1, 2, 3, \dots, 30$  and the absorbing state is 0. Then the canonical form transition probability matrix

is

$$P = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 1/2 & 1/2 & 0 & \cdots & 0 & 0 \\ 1/3 & 1/3 & 1/3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1/30 & 1/30 & 1/30 & \cdots & 1/30 & 0 \end{pmatrix}.$$

The quantity of interest is the expected waiting time until absorption into the state 0. Expressing the first-step analysis compactly in vector-matrix form as

$$(I - T)\mathbf{w} = \mathbf{1},$$

substituting in the values from the transition matrix and solving with a computer, this is  $w_{30} = H_{30} \approx 3.995$ . By calculating the covariance matrix and taking the sum of all entries, the variance of the waiting time from the transient state of all candles lit is approximately 2.383.  $\nabla$

**Example 3.9.** The following example is from the December 22, 2017 Riddler at Fivethirtyeight.com. It concerns a game of chance called Left, Right, Center. In this game, players sit in a circle and start with some number of \$1 bills. Players take turns, in order around the circle, rolling three dice. For each die, if it comes up 1 or 2, the player gives a dollar to the person to the left. If it comes up 3 or 4, the player gives a dollar to the person on the right. And if it comes up 5 or 6, the player puts a dollar in the center. Assume the following: First, if a player has no dollars, then her turn is skipped. Second, if a player has one or two dollars, then the player rolls only one or two dice, respectively. The game ends as soon as only a single person has any money left. How long is the game expected to last for six players each starting with three \$1 bills? For  $X$  players each starting with  $Y$  \$1 bills?

Consider the allocation of the total of \$18 among the 6 players and the center, that is 7 places, as the states of a Markov chain. Using the “stars and bars” argument, choosing  $7 - 1 = 6$  bars from  $18 + 6$  objects the number of states is  $\binom{18+6}{6} = 134,596$ . This also counts all the money in the center as one state which would not strictly be a state of the game. This makes 134,595 actual game states. This is the same as the number of states dividing any number of dollars from 1 to 18 among 6 players, ignoring the money in the center which would be  $\sum_{j=6}^{23} \binom{j}{5} = 134,595$ . This is essentially the conclusion of the hockey-stick identity for binomial coefficients.

The game ends when exactly 1 of the 6 players has any amount of money from \$1 to \$18. That is, there are  $6 \cdot (1 + \cdots + 18) = 6 \cdot 18 \cdot 19/2 = 1026$  terminal states that can be considered as the absorbing states of the game.

The shortest possible game would be for the first 5 players to throw all 5’s and 6’s, leaving the sixth player with the original stake of money. This shortest game would be 5 turns with probability  $(1/27)^5$ .



Dollars	6	7	8	9
3	25.7096	32.3160	38.9660	45.3878
4	31.7890	39.7598	47.3006	55.3804
5	38.3244	47.4416	56.3536	65.4438
6	44.8394	54.9732	65.5688	75.3548

**Table 3.1.** Mean number of turns in 5000 simulations of the game with  $X$  players (columns) each with  $Y$  dollars (rows).

Dollars	6	7	8	9
3	6.546804	7.009249	7.564145	7.898221
4	7.751729	8.176348	8.594918	9.099816
5	8.989401	9.367077	9.878952	10.387840
6	10.16180	10.468601	11.080443	11.654668

**Table 3.2.** Variance of number of turns in 5000 simulations of the game with  $X$  players each with  $Y$  dollars.

Next consider the total number of dollars in the circle at each turn. The expected loss of dollars from the circle to the center at each turn is

$$0 \cdot \left(\frac{2}{3}\right)^3 + 1 \cdot \left(3 \cdot \left(\frac{2}{3}\right)^2 \cdot \left(\frac{1}{3}\right)\right) + 2 \cdot \left(3 \cdot \left(\frac{2}{3}\right) \cdot \left(\frac{1}{3}\right)^2\right) + 3 \cdot \left(\frac{1}{3}\right)^3 = 1.$$

That means it takes should take about 17 turns to end the game. More precisely, consider the lumped system where each state is the number of dollars in the circle, from \$18 to \$1. Let  $D_j$  be the duration of the game from  $j$  dollars with  $j = 1, \dots, 18$ . Then a first-step analysis gives the system of equations  $D_j = (8/27)D_j + (12/27)D_{j-1} + (6/27)D_{j-2} + (1/27)D_{j-3} + 1$ , with  $D_j = 0$  for  $j = 1, 0, -1$ . The solution of this system gives  $D_{18} = 17.3333$  (see the scripts for the solution method) which is consistent with the previous crude estimate.

The number of states and absorbing states are too large to be effectively handled by matrix methods. Although the conceptual set-up of the game is clearly the waiting time until absorption in a Markov chain, simulation seems to be the best way to answer the question. Results of simulating games with 6 to 9 players each starting with 3 to 6 dollars are in Table 3.1 and Table 3.2. The Riddler says the game with  $X$  players each starting with  $Y$  dollars will last  $2(X-2)Y$  turns but does not give a proof. The simulations give means that are roughly consistent with this value.

▽

### 3.9. Chapter Ending Answer

The number of times the Markov chain visits a transient state is a random variable. Let  $Y_{ij}$  denote the number of visits the system makes to transient state  $j$  before reaching an absorbing state, given the system started in transient state  $i$ . Thus,  $Y_{ij}$  is a discrete random variable that can take on any nonnegative integer value.

### 3.10. Chapter Summary

### 3.11. Chapter Summary

#### Key Concepts.

- (1) Let  $\{X_n\}$  be a finite-state absorbing Markov chain with  $a$  absorbing states and  $t$  transient states. Let the  $(a + t) \times (a + t)$  transition probability matrix be  $P$ . Order the states so the absorbing states come first and non-absorbing, i.e. transient, states come last. Then the transition probability matrix has the block-matrix form

$$P = \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix}.$$

Here  $I_a$  is an  $a \times a$  identity matrix,  $A$  is the  $t \times a$  matrix of single-step transition probabilities from the  $t$  transient states to the  $a$  absorbing states,  $T$  is a  $t \times t$  submatrix of single-step transition probabilities among the transient states, and  $0$  is a  $a \times t$  matrix of 0s representing the single-step transition probabilities from absorbing states to transient states.

- (2) The matrix  $N = (I - T)^{-1}$  is the **fundamental matrix** for the absorbing Markov chain. The entries  $N_{ij}$  of this matrix have a probabilistic interpretation. The entries  $N_{ij}$  are the expected number of times the chain started from state  $i$  will be in state  $j$  before ultimate absorption.
- (3) First-step analysis gives a compact expression in vector-matrix form for the waiting time  $\mathbf{w}$  to absorption:

$$(I - T)\mathbf{w} = \mathbf{1}$$

so  $\mathbf{w} = (I - T)^{-1}\mathbf{1}$ .

#### Vocabulary.

- (1) Let  $\{X_n\}$  be a finite-state absorbing Markov chain with  $a$  absorbing states and  $t$  transient states. Let the  $(a + t) \times (a + t)$  transition probability matrix be  $P$ . Order the states so the absorbing states come first and non-absorbing, i.e. transient, states come last. Then  $(P^n)_{ij} \rightarrow 0$  as  $n \rightarrow \infty$  for  $i$  and  $j$  in the transient states, while for  $i$  in the absorbing states,  $P_{ii} = 1$ . Define the **absorption time** as the random variable

$$T = \min \{n \geq 0 : X_n \leq a\}.$$

- (2) The **absorption probability matrix**  $B$  is the probability of starting at state  $i$  and ending at absorbing state  $j$ .
- (3) For a Markov chain with  $a$  absorbing states and  $t$  transient states, if necessary, reorder the states so the absorbing states come first and non-absorbing, i.e. transient, states come last. Then the transition matrix has the canonical form:

$$P = \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix}.$$

The matrix  $N = (I - T)^{-1}$  is the **fundamental matrix** for the absorbing Markov chain.

- (4) The  $N$ th **harmonic number**  $H_N$  is

$$H_N = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \cdots + \frac{1}{N}.$$

**Notation.**

- (1)  $\{X_n\}$  – a finite-state absorbing Markov chain with  $a$  absorbing states and  $t$  transient states.
- (2)  $P$  – the  $(a + t) \times (a + t)$  transition probability matrix.
- (3)  $I_a$  is an  $a \times a$  identity matrix,  $A$  is the  $t \times a$  matrix of single-step transition probabilities from the  $t$  transient states to the  $a$  absorbing states,  $T$  is a  $t \times t$  submatrix of single-step transition probabilities among the transient states, and  $0$  is a  $a \times t$  matrix of 0s representing the single-step transition probabilities from absorbing states to transient states.
- (4)  $i, j, l$  – arbitrary states of the Markov chain
- (5)  $Y_{ij}$  – the number of visits the system makes to transient state  $j$  before reaching an absorbing state, given the system started in transient state  $i$ .
- (6)  $w_i$  – mean time until absorption for transient state  $i$
- (7)  $\mathbf{w}$  – vector of waiting times until absorption for transient states
- (8)  $\mathbf{1}_{ij}^{(m)}$  – indicator random variable if the Markov chain is in transient state  $j$  after  $m$  steps given that it starts in transient state  $i$
- (9)  $\delta_{ij}$  – Kronecker delta function
- (10)  $N = (I - T)^{-1}$  – fundamental matrix
- (11)  $\mathbf{1}$  – vector with all entries 1
- (12)  $D_j$  – Duration of the Left, Right, Center game when  $j$  dollars are in the center.

### 3.12. Sources

The section on covariances is adapted from Carchidi and Higgins [CH17]. The section on first-step analysis is adapted from *Finite Markov Chains* by Kemeny and Snell [KS60]. Other ideas are from *An Introduction to Stochastic Modeling* by Taylor and Karlin citetaylor98-introd-stoch-model and *Random Walks and Electrical Networks* by Doyle and Snell [DS84]. The birthday candle example is adapted from the January 13, 2017 “Riddler” at Fivethirtyeight.com. The two colored balls example is adapted from *Finite Markov Chains* by Kemeny and Snell [KS60]. The four colored balls example is adapted from Lessard The Left-Center-Right game example is from the December 22, 2017 Riddler at Fivethirtyeight.com.

**3.13. Algorithms and Scripts**

```

1 function playerIndex(j)
2   | Modular division to number the players in a circle
3   | return mod  $((j - 1), p) + 1$ 
4 function game(b, p)
5   Initialize the player circle to hold equal number of bills
6   while more than one player has more than one bill do
7     | Current player takes a turn
8     | Move to next player in circle
9     | Increment turns by 1
10  end
11  return turns
12 function turn(p)
13  Get 3 random integers from 1 to 6 into a vector
14  for three places in the vector do
15    | if current player has bills then
16      | if roll (vector entry) is 1 or 2 then
17        | Player to left gets bill, current player loses a bill
18      | end
19      | if roll (vector entry) is 3 or 4 then
20        | Player to right gets bill, current player loses a bill
21      | end
22      | if roll (vector entry) is 5 or 6 then
23        | Center gets bill (don't keep track), current player loses a bill
24      | end
25    | end
26  end
27 return State of players (the bills each player holds)

```

**Algorithm 3:** Supporting functions for Left-Center-Right

**Data:** Number of players, number of starting bills, number of simulations

**Result:** Matrices of mean and variances of game length

```

1 function main()
2   Initialize Mean and Standard Deviation matrices to hold results
3   Initialize number of simulations (5000)
4   for p ← 6 to 9 do
5     for b ← 3 to 6 do
6       Initialize empty vector to hold waiting time for each simulation
7       for i ← 1 to number of simulations do
8         Play game
9         Record results of waiting times for each simulation
10      end
11    end
12  end
13  return Mean, Standard Deviation of Waiting Times

```

**Algorithm 4:** Waiting Time Simulation for Left-Center-Right

R script for Waiting Time in Left-Center-Right.

```

1 player_index <- function(j) {
2   ((j-1) %% player_count) + 1
3 }
4
5 game <- function(bills, player_count){
6
7   turn <- function(player) {
8     rolls <- sample(6, 3, replace=TRUE)
9     for (roll in rolls) {
10      if (players[player] > 0) {      #player has
money
11      to Left      if (roll <= 2) {      #pass dollar
12      players[player_index(player - 1)] =
13      players[player_index(player - 1)]
14      + 1
15      players[player] = players[player] - 1
16      } else if (roll <= 4) {      #pass dollar
to right
17      players[player_index(player + 1)] =
18      players[player_index(player + 1)]
19      + 1
20      players[player] = players[player] - 1
21      } else {      #dollar goes
to center
22      players[player] = players[player] - 1
}
}
}
}

```

```

23     }
24     return(players)
25 }
26
27 players <- rep(bills, player_count)
28 turns <- 1
29 current_player <- 1
30
31 while ( length( players[ players > 0] ) > 1 ) {
32     players <- turn(current_player)
33     current_player <- player_index(current_player +
1)
34     turns <- turns + 1
35 }
36
37 return(turns)
38 }
39
40 M <- matrix(0, 4, 4)
41 V <- matrix(0, 4, 4)
42 simulations <- 5000
43
44 for (player_count in c(6:9)) {
45     for (bills in c(3:6)) {
46
47         sim_results <- c()
48         for (i in 1:simulations) {
49             sim_results <- c( sim_results, game(bills,
player_count) )
50         }
51
52         M[player_count-5, bills-2] <- mean(sim_results)
53         V[player_count-5, bills-2] <- sd(sim_results)
54     }
55 }

```

### 3.14. Problems to Work for Understanding

Chapter 3: Waiting Time to Absorption.

3.1: A law firm employs three types of lawyers: junior lawyers, senior lawyers, and partners. During a given year, there is probability 0.15 of promoting a junior lawyer to senior lawyer and probability 0.5 that the junior lawyer will leave the firm. There is probability 0.20 of promoting the senior lawyer to partner and probability 0.10 that the senior lawyer will leave the firm. Finally,

there is probability 0.05 that a partner will leave the firm, see Table 3.3. The firm never demotes a lawyer or a partner.

	leave firm	junior lawyer	senior lawyer	partner
leave firm	1	0	0	0
junior lawyer	0.05	0.80	0.15	0
senior lawyer	0.10	0	0.70	0.20
partner	0.05	0	0	0.95

**Table 3.3.** The law firm transition probabilities

- (1) What is the average number of years that a newly hired junior lawyer stays with the firm?
- (2) What is the variance of the number of years a newly hired junior lawyer stays with the firm?

3.2: Consider the random walk of a particle along a straight line from  $-4$  to  $4$  with probability  $2/3$  of moving to the right and probability  $1/3$  of moving to the left. The absorbing boundary states are  $-4$  and  $4$ . Compute the vector of variances of waiting times until absorption using Theorem 3.3. Compare the result with the variance computed in the text for the walk started at  $0$ , using the sum of the entries in the covariance matrix.

3.3: In a small pond there are eleven lily pads in a row labeled  $0$  through  $10$ . A frog is sitting on pad  $1$ . When the frog is on pad  $N$ ,  $0 < N < 10$ , it will jump to pad  $N - 1$  with probability  $\frac{N}{10}$  and to pad  $N + 1$  with probability  $1 - \frac{N}{10}$ . Each jump is independent of the previous jumps. If the frog reaches pad  $0$  it will be eaten by a patiently waiting snake. If the frog reaches pad  $10$  it will exit the pond, never to return. What is the probability that the frog will escape being eaten by the snake?

3.4: A frog sitting at the point  $(1, 2)$  begins a sequence of jumps, where each jump is parallel to one of the coordinate axes and has length  $1$ , and the direction of each jump (up, down, right, or left) is chosen independently at random. The sequence ends when the frog reaches a side of the square with vertices  $(0, 0)$ ,  $(0, 4)$ ,  $(4, 4)$ , and  $(4, 0)$ . What is the probability that the sequence of jumps ends on a vertical side of the square?

3.5: Consider three urns A, B, and C containing  $a$ ,  $b$  and  $c$  balls respectively. Pick an urn at random, each being equally likely, and move a ball from it to one of the other two urns, each being equally likely. The game ends when one of the three urns becomes empty. Derive the mean duration of the game.

3.6: Use mathematical induction to show

$$P^m = \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix}^{m-1} \begin{pmatrix} I_a & 0 \\ A & T \end{pmatrix} = \begin{pmatrix} I_a & 0 \\ (I_t + T + T^2 + \dots + T^{m-1})A & T^m \end{pmatrix}.$$

- 3.7: (a) Use computer software to show the transient state transition probability matrix  $T$  in the random walk example has induced 2-norm (or operator norm) less than one for  $p = 1/2$  and  $p = 2/3$ .

- (b) Use computer software to show the transient state transition probability matrix  $T$  in the birthday candle example with  $N = 5$ , has induced 2-norm (or operator norm) less than 1.
- (c) Use computer software to show the transient state transition probability matrix  $T$  in the two unpainted balls example has induced 2-norm (or operator norm) less than 1.
- (d) (Mathematicians only) Show that if  $T$  is irreducible and row substochastic, with at least one row having sum less than 1, then the induced 2-norm (or operator norm) of  $T$  is less than 1,  $\|T\| < 1$ .
- (e) Use computer software to show the transient state transition probability matrix  $T$  in the four painted balls example has induced 2-norm (or operator norm) *greater* than 1. Explain why the previous theorem is not violated. Nevertheless, show the eigenvalues of the matrix are all less than 1, so  $T$  is contractive and  $(I - T)^{-1}$  still exists.

3.8: Show  $NT = (I_t - T)^{-1}T = N - I_t$

3.9: Under the assumption the induced 2-norm (or operator norm) of  $T$  is less than 1,  $\|T\| < 1$  prove that

$$\sum_{\nu=0}^{\infty} (T^\nu) = (I - T)^{-1}.$$

3.10: For the birthday candle problem, prove by induction that the waiting time with  $N$  candles is the  $N$ th harmonic number  $H_N$ .





## Standard Examples of Markov Chains

This chapter shows a wide variety of standard examples to illustrate simple Markov chains: sums of independent random variables, random walks on finite and infinite state spaces, and urn models. Each Markov chain is explained with their elementary properties and classifications.

Mathematically Mature: contains mathematics beyond calculus with proofs.

### 4.1. Chapter Starter Question

Give an example from elementary probability of a simple Markov chain.

### 4.2. State Homogeneous Markov Chains

**Example 4.1.** The **simple state homogeneous Markov chain** is a Markov chain representation of drawing independent random samples from a distribution. Let  $\xi$  denote a discrete-valued random variable with possible values as the nonnegative integers  $\mathbb{P}[\xi = i] = p_i$ , where  $p_i \geq 0$  and  $\sum_{i=1}^{\infty} p_i = 1$ . Let  $\xi_1, \xi_2, \xi_3, \dots$  be independent observations of  $\xi$ . Then consider the process  $X_i, n = 1, 2, 3, \dots$  defined by  $X_n = \xi_n$ . The transition probability matrix of this state homogeneous Markov chain is schematically

$$P = \begin{pmatrix} p_1 & p_2 & p_3 & \dots \\ p_1 & p_2 & p_3 & \dots \\ p_1 & p_2 & p_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

If  $p_i = 0$  for  $i > k$ , then the state space of the Markov chain is finite, with corresponding  $k \times k$  finite transition probability matrix.

In this example, make the sensible assumption that  $0 < p_i < 1$  for the set of states, either finite or infinite, so that only states with a probability of appearing

are considered. The stationary distribution is  $(p_1, p_2, p_3, \dots)$ . Note that  $P^n = P$ . With the assumption, this Markov chain is aperiodic, each state is accessible and all states communicate, recurrent, and has no absorbing states.

This Markov chain is equivalent to independent samples from the distribution  $\mathbb{P}[\xi = i] = p_i$ .  $\triangle$

**Example 4.2. Sums of independent random variables as Markov chains** arise from successive partial sums  $\eta_n$  of the random variables of the independent observations of the  $\xi_i$

$$\eta_n = \xi_1 + \xi_2 + \xi_3 + \dots + \xi_n$$

with  $\eta_0 = 0$  by definition. The entries of the probability transition matrix are defined by

$$\begin{aligned} \mathbb{P}[X_{n+1} = j \mid X_n = i] \\ &= \mathbb{P}[\xi_1 + \xi_2 + \xi_3 + \dots + \xi_n + \xi_{n+1} = j \mid \xi_1 + \xi_2 + \xi_3 + \dots + \xi_n = i] \\ &= \mathbb{P}[\xi_{n+1} = j - i] \end{aligned}$$

assuming the independence of the  $\xi_i$ . Schematically the probability transition matrix is

$$P = \begin{pmatrix} p_1 & p_2 & p_3 & p_4 & \dots \\ 0 & p_1 & p_2 & p_3 & \dots \\ 0 & 0 & p_1 & p_2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

If the random variables  $\xi$  assumes both positive and negative integers, then the possible values of the partial sums  $\eta_n$  will be contained in the set of all integers. Then let the state space be  $\mathbb{Z}$ . Letting  $\mathbb{P}[\xi = i] = p_i$ ,  $i \in \mathbb{Z}$ , with  $p_i \geq 0$ ,  $\sum_{i=-\infty}^{\infty} p_i = 1$ . Then schematically the probability transition matrix is

$$P = \begin{pmatrix} \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & p_{-1} & p_0 & p_1 & p_2 & p_3 & p_4 & \cdots \\ \cdots & p_{-2} & p_{-1} & p_0 & p_1 & p_2 & p_3 & \cdots \\ \cdots & p_{-3} & p_{-2} & p_{-1} & p_0 & p_1 & p_2 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

This Markov chain is quite general and so special cases will be considered as examples of the various characteristics of Markov chains.  $\triangle$

### 4.3. Random Walks as Markov Chains

**Example 4.3. Random Walk with Absorbing Boundaries**

In **random walk with boundaries** the state space is the finite set of integers  $\{0, 1, 2, 3, \dots, k\}$ . A particle at site  $i$  can stay at  $i$  with probability  $r_i$  or move to adjacent site  $i + 1$  with probability  $p_i$  and to adjacent site  $i - 1$  with probability  $q_i$  with  $p_i + r_i + q_i = 1$ . The transitions at the boundaries 0 and  $k$  get special

consideration. The transition probability matrix in general is

$$P = \begin{pmatrix} r_0 & p_0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ q_1 & r_1 & p_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & q_2 & r_2 & p_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & q_3 & r_3 & p_3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & q_k & r_k \end{pmatrix}.$$

If  $r_0 = r_k = 1$  the particle reaches sites 0 or  $k$ , then it stays at that site with probability 1. This is a **random walk with absorbing boundaries**. In a common special case, the transition probabilities do not depend on  $i$  and  $r_i = 0$ . The transition probability matrix is

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ q & 0 & p & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & q & 0 & p & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & q & 0 & p & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}.$$

This is also the Markov chain for the gambler's ruin.

All states are accessible from states  $i$  for  $0 < i < k$ , but because of the absorbing boundaries, not all states communicate. The transient states are  $1, 2, \dots, k-1$  and the absorbing states are 0 and  $k$ . Therefore, it does not make sense to consider any stable distributions.  $\triangle$

**Example 4.4.** *Random Walk with Reflecting Boundaries*

In a **random walk with reflecting boundaries** the state space is the finite set of integers  $\{0, 1, 2, 3, \dots, k\}$ . A particle at site  $i$  with  $1 < i < k-1$  moves to adjacent site  $i+1$  with probability  $p$  and to adjacent site  $i-1$  with probability  $q$  with  $p+q=1$ . If the particle reaches sites 0 or  $k$ , then at the next step it is at 1 or  $n-1$  respectively with probability 1. The transition probability matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ q & 0 & p & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & q & 0 & p & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}.$$

For this transition probability matrix  $P$  there is a probability distribution  $\pi$  such that  $\pi P = \pi$ . It is not strictly true that the Markov chain has a stationary distribution because the chain has period 2. This can be fixed by embedding this random walk in a *lazy random walk* where, given  $X_{n-1}$ , first choose to remain at  $X_{n-1}$  with probability  $\frac{1}{2}$ . Alternatively, with probability  $\frac{1}{2}$  choose to move to  $X_n$  selected with probability  $q$  and  $p$  from the left and right nodes adjacent to  $x_{n-1}$ . The original chain is periodic with period 2, but the associated lazy random walk is aperiodic. All states are accessible and all states communicate. This Markov

chain has no transient states and all states are recurrent. The Markov chain has no absorbing states.

**Random Walk on a Circle.** In **random walk on a circle** the state space is the finite set of integers  $\{0, 1, 2, 3, \dots, k\}$ . A particle at site  $i$  with  $1 < i < k - 1$  moves to adjacent site  $i + 1$  with probability  $p$  and to adjacent site  $i - 1$  with probability  $q$  with  $p + q = 1$ . If the particle reaches site 0, then at the next step it is at  $k$  or 1 with probability  $q$  or  $p$  respectively. If the particle reaches site  $k$ , then at the next step it is at  $k - 1$  or 0 with probability  $q$  or  $p$  respectively. The transition probability matrix is

$$P = \begin{pmatrix} 0 & p & 0 & 0 & 0 & \cdots & 0 & 0 & q \\ q & 0 & p & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & q & 0 & p & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ p & 0 & 0 & 0 & 0 & \cdots & 0 & q & 0 \end{pmatrix}.$$

This is also a random walk with state space  $\mathbb{Z}_{k+1}$ .

This Markov chain has a stationary distribution

$$(1/(k+1), 1/(k+1), \dots, 1/(k+1))$$

(subject to the embedding into a lazy random walk as in the previous example.) The original chain is periodic with period 2. All states are accessible and all states communicate. This Markov chain has no transient states and all states are recurrent. This Markov chain has no absorbing states.  $\triangle$

**Example 4.5. Unbiased Walk on Integers**

In **unbiased random walk on the integers**, also called symmetric random walk, the state space is the infinite set of integers  $\mathbb{Z}$ . A particle at site  $i$  with  $i$  moves to adjacent site  $i + 1$  with probability  $1/2$  and to adjacent site  $i - 1$  with probability  $1/2$ . The transition probability is

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

Because this Markov chain has an infinite state space, it does not make sense to consider a stable distribution. The chain is periodic with period 2. All states are accessible and all states communicate. It is a deep theorem that the Markov chain has no transient states and all states are recurrent, see for example [Les05, Section 13.2]. Therefore, this is an example of an infinite state space Markov chain that is also recurrent. This Markov chain has no absorbing states.  $\triangle$

**Example 4.6. Biased Walk on Integers**

In **biased random walk on the integers** the state space is the infinite set of integers  $\mathbb{Z}$ . A particle at site  $i$  with  $i$  moves to adjacent site  $i + 1$  with probability  $p$  and to adjacent site  $i - 1$  with probability  $q$  with  $p \neq q$  and  $p + q = 1$ . The

transition probability is

$$p_{ij} = \begin{cases} p & \text{if } j = i - 1, \\ q & \text{if } j = i + 1, \\ 0 & \text{if } j \neq i - 1, i + 1. \end{cases}$$

Because this Markov chain has an infinite state space, it does not make sense to consider a stable distribution. The chain is periodic with period 2. All states are accessible and all states communicate. It is a substantial theorem that all states are transient states and no states are recurrent, see for example [Les05, Section 13.4]. Therefore, this is an example of an infinite state space Markov chain that is not recurrent. This Markov chain has no absorbing states.  $\triangle$

**Example 4.7. Random Walks on Graphs**

Each of these examples of a Markov chain is a specific case of a more general **random walk on a graph**. A **graph** is a finite or infinite set of nodes, also called vertices,  $\{v_1, v_2, \dots, v_k\}$ , and an associated collection of edges  $\{v_{ij}, 1 \leq i, j \leq n\}$ . There need not be an edge between two vertices. If there is a connection between vertices  $v_i$  and  $v_j$ , then  $v_j$  is in the neighborhood  $N(v_i)$  of  $v_i$ . A particle at vertex  $v_i$  will move to a vertex  $v_j$  in the neighborhood  $N(v_i)$  with probability  $p_{ij}$  and may stay at  $v_i$  with probability  $p_{ii}$ , where  $\sum_{j \in \{i\} \cup N(v_i)} p_{ij} = 1$ .

For a small specific example, consider the  $3 \times 3$  square lattice graph in Figure 4.1. The graph has 9 vertices with 10 edges between nearest lattice neighbors. If a vertex has  $n$  edges then the probability of moving to a neighboring edge or staying at the vertex is  $\frac{1}{n+1}$  uniformly. The random walk on this graph is often colorfully characterized as a frog hopping among lily pads or a bug leaping among plants. The transition probability matrix for this graph random walk is

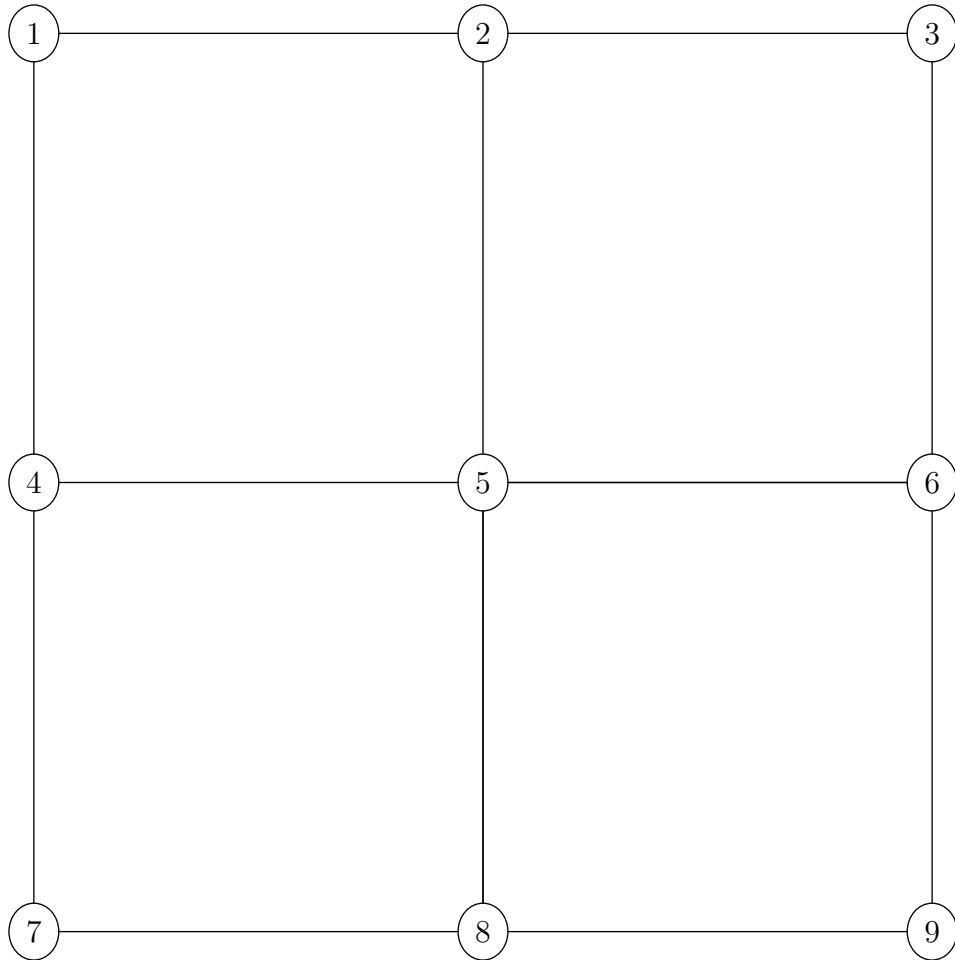
$$\begin{pmatrix} 1/3 & 1/3 & 0 & 1/3 & 0 & 0 & 0 & 0 & 0 \\ 1/4 & 1/4 & 1/4 & 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 1/3 & 0 & 0 & 1/3 & 0 & 0 & 0 \\ 1/4 & 0 & 0 & 1/4 & 1/4 & 0 & 1/4 & 0 & 0 \\ 0 & 1/5 & 0 & 1/5 & 1/5 & 1/5 & 0 & 1/5 & 0 \\ 0 & 0 & 1/4 & 0 & 1/4 & 1/4 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 1/3 & 0 & 0 & 1/3 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 & 1/4 & 1/4 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 1/3 & 0 & 1/3 & 1/3 \end{pmatrix}.$$

This Markov chain has a stationary distribution

$$\pi = (\frac{1}{11}, \frac{4}{33}, \frac{1}{11}, \frac{4}{33}, \frac{5}{33}, \frac{4}{33}, \frac{1}{11}, \frac{4}{33}, \frac{1}{11}).$$

The chain is aperiodic. All states are accessible and all states communicate. This Markov chain has no transient states and all states are recurrent. This Markov chain has no absorbing states.

The stationary distribution  $\pi$  is unique and the chain converges to  $\pi$  as  $n \rightarrow \infty$ . Later sections will use this Markov chain as an example about quantitative rates of convergence, that is, how large  $n$  must be to make the chain sufficiently close to  $\pi$ .  $\nabla$



**Figure 4.1.** A  $3 \times 3$  square lattice graph with uniform transition probabilities.

#### 4.4. Urn Models

**Example 4.8.** *Ehrenfest Urn Model*

The physicist P. Ehrenfest proposed the following model for statistical mechanics and kinetic theory. The motivation is diffusion through a membrane. Two urns labeled  $A$  and  $B$  contain a total of  $k$  balls. In the **Ehrenfest urn model** a ball is selected at random with all selections equally likely, and moved from the urn it is in to the other urn. The state at each time is the number of balls in the urn  $A$ ,

from 0 to  $k$ . Then the transition probability matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ \frac{1}{k} & 0 & 1 - \frac{1}{k} & 0 & \cdots & 0 & 0 \\ 0 & \frac{2}{k} & 0 & 1 - \frac{2}{k} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1/k \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}.$$

The balls fluctuate between the two containers with a drift from the one with the larger number of balls to the one with the smaller numbers.

A stationary distribution for this Markov chain has entry  $\pi_i = \binom{k}{i}/2^k$  subject to the embedding into a lazy Markov chain as in the previous examples. (See the exercises.) This is the binomial distribution on  $k$ , so that for large  $k$ , this can be approximated with the normal distribution. This conclusion is plausible given the physical origin of the Markov chain as a model for diffusion. All states are accessible and all states communicate. The chain is periodic with period 2 unless it is embedded in a lazy Markov chain. All states are recurrent with no transient states. This Markov chain has no absorbing states.

**An Alternate Ehrenfest Urn Model.** Two urns labeled  $A$  and  $B$ , contain a total of  $k$  balls. A ball is selected at random with all selections equally likely. Then an urn is selected, urn  $A$  with probability  $p$  and urn  $B$  with probability  $q = 1 - p$  and the ball is moved to that urn. The state at each time is the number of balls in the urn  $A$ , from 0 to  $N$ . Then the transition probability matrix is

$$P = \begin{pmatrix} q & p & 0 & 0 & \cdots & 0 & 0 \\ \frac{1}{k}q & \frac{1}{k}p + \left(1 - \frac{1}{k}\right)q & \left(1 - \frac{1}{k}\right)p & 0 & \cdots & 0 & 0 \\ 0 & \frac{2}{k}q & \frac{2}{k}p + \left(1 - \frac{2}{k}\right)q & \left(1 - \frac{2}{k}\right)p & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & q & p \end{pmatrix}.$$

A stationary distribution for this Markov chain exists, but depends on  $p$ ,  $i$ , and  $k$  in a more complicated relationship than in the previous example. All states are accessible and all states communicate. The chain is aperiodic. All states are recurrent and there are no transient states. This Markov chain has no absorbing states.  $\triangle$

**Example 4.9. Another Ehrenfest Urn Model**

Two urns labeled  $A$  and  $B$  contain a total of  $k$  balls. At time  $t$  there  $i$  balls in urn  $A$ . At time  $t + 1$  an urn is selected, urn  $A$  with probability  $i/k$  and urn  $B$  with probability  $(k - i)/k$ . Then independently a ball is selected from urn  $A$  with probability  $p$  or from urn  $B$  with probability  $q = 1 - p$  and placed in the previously selected urn. The state at each time is the number of balls in the urn  $A$ , from 0 to



$k$ . Then the transition probability matrix is

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \frac{k-1}{k}p & \frac{k-1}{k}q + \left(\frac{1}{k}\right)p & \left(\frac{1}{k}\right)q & 0 & \cdots & 0 & 0 \\ 0 & \frac{k-2}{k}p & \left(1 - \frac{2}{k}\right)q + \frac{2}{k}p & \left(\frac{2}{k}\right)p & \cdots & 0 & 0 \\ 0 & 0 & \frac{k-3}{k}p & \left(\frac{k-3}{k}\right)q + \frac{3}{k}p & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

States 1 through  $k-1$  communicate while states 0 and  $k$  are absorbing. States 1 to  $k-1$  are transient states. The chain is aperiodic.  $\triangle$

**Example 4.10.** *Yet Another Generalized Ehrenfest Urn Model*

Two urns labeled  $A$  and  $B$ , contain a total of  $k$  balls. At time  $t$  there  $i$  balls in urn  $A$ . At time  $t+1$  an urn is selected, urn  $A$  with probability  $i/k$  and urn  $B$  with probability  $(k-i)/k$ . Then independently a ball is selected from urn  $A$  with probability  $i/k$  or from urn  $B$  with probability  $(k-i)/k$  and placed in the previously selected urn. The state at each time is the number of balls in the urn  $A$ , from 0 to  $k$ . Then the transition probability matrix is

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \frac{1 \cdot (k-1)}{k^2} & \frac{1^2}{k^2} + \frac{(k-1)^2}{k^2} & \frac{(k-1) \cdot 2}{k^2} & 0 & \cdots & 0 & 0 \\ 0 & \frac{2 \cdot (k-2)}{k^2} & \frac{2^2}{k^2} + \frac{(k-2)^2}{k^2} & \frac{(k-2) \cdot 2}{k^2} & \cdots & 0 & 0 \\ 0 & 0 & \frac{3 \cdot (k-3)}{k^2} & \frac{3^2}{k^2} + \frac{(k-3)^2}{k^2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

States 1 through  $k-1$  communicate while states 0 and  $k$  are absorbing. States 1 to  $k-1$  are transient states. The chain is periodic with period 1.  $\triangle$

#### 4.5. Chapter Ending Answer

A standard example from elementary probability theory that is also a Markov chain is the sequence of partial sums of a sequence of independent identically distributed random variables. This has the natural interpretation as a random walk, also a simple example of a Markov chain.

#### 4.6. Chapter Summary

**Key Concepts.**

- (1) A wide variety of standard examples illustrate simple Markov chains: sums of independent random variables, random walks on finite and infinite state spaces, random walks on graphs, and urn models.
- (2) Random walks on finite state spaces can have absorbing or reflecting boundaries, or even be circular. Different boundary conditions lead to different Markov chains.

- (3) The physicist P. Ehrenfest proposed an urn model for statistical mechanics and kinetic theory. The motivation is diffusion through a membrane. Two urns labeled  $A$  and  $B$ , contain a total of  $N$  balls and the state is the number of balls in one urn. Different urn and ball selections lead to different Markov chains.

### Vocabulary.

- (1) The **simple state homogeneous Markov chain** is a Markov chain representation of drawing independent random samples from a distribution.
- (2) **Sums of independent random variables as Markov chains** arise from successive partial sums  $\eta_n$  of the random variables of the independent observations of the  $\xi_i$ .
- (3) In **random walk with boundaries** the state space is the finite set of integers  $\{0, 1, 2, 3, \dots, k\}$ . A particle at site  $i$  can stay at  $i$  with probability  $r_i$  or move to adjacent site  $i+1$  with probability  $p_i$  and to adjacent site  $i-1$  with probability  $q_i$  with  $p_i + r_i + q_i = 1$ . The transitions at the boundaries 0 and  $k$  get special consideration.
- (4) In a **random walk with absorbing boundaries**,  $r_0 = r_n = 1$  so as the particle reaches sites 0 or  $n$ , then it stays at that site with probability 1.
- (5) In a **random walk with reflecting boundaries** if the particle reaches sites 0 or  $n$ , then at the next step it is at 1 or  $n-1$  respectively with probability 1.
- (6) In a **random walk on a circle** if the particle reaches site 0, then at the next step it is at  $n$  or 1 with probability  $q$  or  $p$  respectively. If the particle reaches site  $n$ , then at the next step it is at  $n-1$  or 1 with probability  $q$  or  $p$  respectively.
- (7) In **unbiased random walk on the integers**, also called symmetric random walk, the state space is the infinite set of integers  $\mathbb{Z}$ . A particle at site  $i$  moves to adjacent site  $i+1$  with probability  $1/2$  and to adjacent site  $i-1$  with probability  $1/2$ .
- (8) In **biased random walk on the integers** the state space is the infinite set of integers  $\mathbb{Z}$ . A particle at site  $i$  moves to adjacent site  $i+1$  with probability  $p$  and to adjacent site  $i-1$  with probability  $q$  with  $p \neq q$  and  $p + q = 1$ .
- (9) A **graph** is a finite or infinite set of nodes, also called vertices,  $\{v_1, v_2, \dots, v_n\}$ , and an associated collection of edges  $\{v_{ij}, 1 \leq i, j \leq n\}$ . There need not be an edge between any two vertices, but if there is a connection between vertices  $v_i$  and  $v_j$ , then  $v_j$  is in the neighborhood  $N(v_i)$  of  $v_i$ .
- (10) In the more general **random walk on a graph** a particle at vertex  $v_i$  will move to a vertex  $v_j$  in the neighborhood  $N(v_i)$  with probability  $p_{ij}$  and may stay at  $v_i$  with probability  $p_{ii}$ , where  $\sum_{k \in \{i\} \cup N(v_i)} p_{ik} = 1$ .
- (11) In the **Ehrenfest urn model** a ball is selected at random from one of two urns with all selections equally likely, and moved from the urn it is in to the other urn. The state from 0 to  $N$  at each time is the number of balls in a fixed urn.

**Notation.**

- (1)  $i, j, l$  – arbitrary states of the Markov chain
- (2)  $\xi$  – a discrete-valued random variable with possible values as the nonnegative integers  $\mathbb{P}[\xi = i] = p_i$
- (3)  $\xi_1, \xi_2, \xi_3, \dots$  – independent observations of  $\xi$
- (4)  $X_n$  – Markov chain with transition probability matrix  $P$
- (5) successive partial sums  $\eta_n$  of the random variables of the independent observations of the  $\xi_i$
- (6)  $p_i, q_i, r_i$  – A particle at site  $i$  can stay at  $i$  with probability  $r_i$  or move to adjacent site  $i+1$  with probability  $p_i$  and to adjacent site  $i-1$  with probability  $q_i$  with  $p_i + r_i + q_i = 1$ .
- (7)  $p, q = 1 - p$  – simple Bernoulli probabilities
- (8)  $n, t$  – time steps or periods of the Markov chain
- (9)  $\pi$  – stationary distribution for a Markov chain
- (10)  $k$  – related to the number of states of the Markov chain ( $k+1$  states if there is a 0 state)

**4.7. Sources**

This section is adapted from: *A First Course in Stochastic Processes*, by S. Karlin and H. Taylor, Chapter 2, pages 45–80, [KT75]; with more information and ideas from *Problems in Probability Theory, Mathematical Statistics and Theory of Random Functions* by A. A. Svesnikov, Chapter VIII, pages 231–274, [Sve68]

#### 4.8. Outside Readings and Links:

#### 4.9. Algorithms and Scripts

**Data:** State names and probability transition matrix

**Result:** Information about a simple Markov chain

- 1 *Initialization and sample paths*
- 2 Load Markov chain library
- 3 Set state names, set transition probability matrix, set start state
- 4 Set an example length and create a sample path of example length
- 5 Create a second sample path of example length
- 6 *Simulation of stationary distribution and comparison to theoretical*
- 7 Set a long path length, and a transient time
- 8 Create a long sample path
- 9 Slice the long sample path from the transient time to the end
- 10 In the slice count the appearance of each state
- 11 Store in an empirical array
- 12 Compute the theoretical stable array
- 13 **return** *Stable distribution and theoretical stable distribution*

**Algorithm 5:** Markov chain simulation.

**R:** R script for Random Walk with Absorbing Boundaries.

```

1 library(markovchain)
2
3 N <- 7
4 stateNames <- as.character( 0:N )
5 transMatrix <- matrix(0, N+1,N+1)
6 transMatrix[1,1] <- 1
7 transMatrix[N+1, N+1] <- 1
8 for (row in 2:N) { #row 2 is state 1, row 7 is state
9   transMatrix[row, row-1] <- 1/2
10  transMatrix[row, row+1] <- 1/2
11 }
12 startState <- "3"
13
14 absorbingbdy <- new("markovchain", transitionMatrix=
15   transMatrix,
16   states=stateNames, name="
17   AbsorbingBdy")
18 print(absorbingbdy)
19
20 print( summary(absorbingbdy) )
21
22 pathLength <- 10
23 path <- rmarkovchain(n=pathLength,

```

```

22                                     object = absorbingbdy, t0
    = startState)
23 cat("A sample starting from ", startState, path, "\n"
    )
24 path <- rmarkovchain(n=pathLength,
25                                     object = absorbingbdy, t0
    = startState)
26 cat("Another sample starting from ", startState, path
    , "\n")
27
28 if ( length( transientStates(absorbingbdy) ) == 0 ) {
29     largeN <- 1000; startStable <- 100
30     path <- rmarkovchain(n=largeN,
31                                     object = absorbingbdy, t0
    = startState)
32     stablePattern <- path[startStable:largeN]
33     empiricalStable <- rep(0, N+1)
34     for (i in seq_along(stateNames)) {
35         empiricalStable[i] <- mean( stablePattern ==
    (i-1) )
36     }
37     theorStable <- steadyStates(absorbingbdy)
38     cat("Empirical stable distribution: ",
    empiricalStable, "\n")
39     cat("Theoretical stable distribution: ",
    theorStable, "\n")
40 }

```

R script for Random Walk with Reflecting Boundaries.

```

1 library(markovchain)
2
3 N <- 7
4 stateNames <- as.character( 0:N )
5 transMatrix <- matrix(0, N+1,N+1)
6 transMatrix[1,2] <- 1
7 transMatrix[N+1, N] <- 1
8 for (row in 2:N) { #row 2 is state 1, row 7 is state
    6
9     transMatrix[row, row-1] <- 1/2
10    transMatrix[row, row+1] <- 1/2
11 }
12 startState <- "3"
13
14 reflectingbdy <- new("markovchain", transitionMatrix=
    transMatrix,

```

```

15         states=stateNames, name="
    ReflectingBdy")
16 print(reflectingbdy)
17
18 print( summary(reflectingbdy) )
19
20 pathLength <- 10
21 path <- rmarkovchain(n=pathLength,
22                     object = reflectingbdy,
23                     t0 = startState)
24 cat("A sample starting from ", startState, path, "\n"
25     )
26 path <- rmarkovchain(n=pathLength,
27                     object = reflectingbdy,
28                     t0 = startState)
29 cat("Another sample starting from ", startState, path
30     , "\n")
31
32 if ( length( transientStates( reflectingbdy) ) == 0 )
33 {
34     largeN <- 1000; startStable <- 100
35     path <- rmarkovchain(n=largeN,
36                         object = reflectingbdy, t0 =
37                         startState)
38     stablePattern <- path[startStable:largeN]
39     empiricalStable <- rep(0, N+1)
40     for (i in seq_along(stateNames)) {
41         empiricalStable[i] <- mean( stablePattern ==
42         (i-1) )
43     }
44     theorStable <- steadyStates(reflectingbdy)
45     cat("Empirical stable distribution: ",
46         empiricalStable, "\n")
47     cat("Theoretical stable distribution: ",
48         theorStable, "\n")
49 }

```

R script for Random Walk on a Circle.

```

1 library(markovchain)
2
3 N <- 7
4 stateNames <- as.character( 0:N )
5 transMatrix <- matrix(0, N+1,N+1)
6 transMatrix[1,2] <- 1/2; transMatrix[1,N+1] <- 1/2
7 transMatrix[N+1, N] <- 1/2; transMatrix[N+1,1] <- 1/2

```

```

8 for (row in 2:N) { #row 2 is state 1, row 7 is state
9   transMatrix[row, row-1] <- 1/2
10  transMatrix[row, row+1] <- 1/2
11 }
12 startState <- "3"
13
14 walkcircle <- new("markovchain", transitionMatrix=
15   transMatrix,
16   states=stateNames, name="Walkcircle"
17 )
18 print(walkcircle)
19
20 pathLength <- 10
21 path <- rmarkovchain(n=pathLength,
22   object = walkcircle, t0 =
23   startState)
24 cat("A sample starting from ", startState, path, "\n"
25 )
26 path <- rmarkovchain(n=pathLength,
27   object = walkcircle, t0 =
28   startState)
29 cat("Another sample starting from ", startState, path
30 , "\n")
31
32 if ( length( transientStates(walkcircle) ) == 0 ) {
33   largeN <- 1000; startStable <- 100
34   path <- rmarkovchain(n=largeN,
35     object = walkcircle, t0 =
36     startState)
37   stablePattern <- path[startStable:largeN]
38   empiricalStable <- rep(0, N+1)
39   for (i in seq_along(stateNames)) {
40     empiricalStable[i] <- mean( stablePattern ==
41       (i-1) )
42   }
43   theorStable <- steadyStates(walkcircle)
44   cat("Empirical stable distribution: ",
45     empiricalStable, "\n")
46   cat("Theoretical stable distribution: ",
47     theorStable, "\n")
48 }

```

R script for Ehrenfest Urn Model.

```

1 library(markovchain)
2
3 N <- 7
4 stateNames <- as.character( 0:N )
5 transMatrix <- matrix(0, N+1,N+1)
6 transMatrix[1,2] <- 1
7 transMatrix[N+1, N] <- 1
8 for (row in 2:N) { #row 2 is state 1, row 7 is state
9   transMatrix[row, row-1] <- (row-1)/N
10   transMatrix[row,row+1] <- (N-(row-1))/N
11 }
12 startState <- "3"
13
14 ehrenfest1 <- new("markovchain", transitionMatrix=
15   transMatrix,
16   states=stateNames, name="Ehrenfest1"
17 )
18 print(ehrenfest1)
19
20 pathLength <- 10
21 path <- rmarkovchain(n=pathLength,
22   object = ehrenfest1, t0 =
23   startState)
24 cat("A sample starting from ", startState, path, "\n"
25 )
26 path <- rmarkovchain(n=pathLength,
27   object = ehrenfest1, t0 =
28   startState)
29 cat("Another sample starting from ", startState, path
30 , "\n")
31
32 if ( length( transientStates(ehrenfest1) ) == 0 ) {
33   largeN <- 1000; startStable <- 100
34   path <- rmarkovchain(n=largeN,
35     object = ehrenfest1, t0 =
36     startState)
37   stablePattern <- path[startStable:largeN]
38   empiricalStable <- rep(0, N+1)
39   for (i in seq_along(stateNames)) {
40     empiricalStable[i] <- mean( stablePattern ==
41     stateNames[i] )
42   }
43   theorStable <- steadyStates(ehrenfest1)

```



```

38   cat("Empirical stable distribution: ",
      empiricalStable, "\n")
39   cat("Theoretical stable distribution: ",
      theorStable, "\n")
40 }

```

R script for alternative Ehrenfest Urn Model.

```

1  library(markovchain)
2
3  N <- 7; p <- 1/2; q <- 1 - p;
4  stateNames <- as.character( 0:N )
5  transMatrix <- matrix(0, N+1,N+1)
6  transMatrix[1,1] <- q
7  transMatrix[1,2] <- p
8  transMatrix[N+1, N ] <- q
9  transMatrix[N+1, N+1] <- p
10 for (row in 2:N) {
11   transMatrix[row, row-1] <- ((N-(row-1))/N)*p
12   transMatrix[row,row] <- ((N-(row-1))/N)*q + ((row
13   -1)/N)*p
14   transMatrix[row,row+1] <- ((row-1)/N)*q
15 }
16 startState <- "3"
17 ehrenfest2 <- new("markovchain", transitionMatrix=
18   transMatrix,
19   states=stateNames, name="Ehrenfest2"
20 )
21 print(ehrenfest2)
22
23 print( summary(ehrenfest2) )
24
25 pathLength <- 10
26 path <- rmarkovchain(n=pathLength,
27   object = ehrenfest2, t0 =
28   startState)
29 cat("A sample starting from startState ", startState,
30   path, "\n")
31 path <- rmarkovchain(n=pathLength,
32   object = ehrenfest2, t0 =
33   startState)
34 cat("Another sample starting from ", startState, path
35   , "\n")
36
37 if ( length( transientStates(ehrenfest2) ) == 0 ) {
38   largeN <- 1000; startStable <- 100
39 }

```

```

33   path <- rmarkovchain(n=largeN,
34                       object = ehrenfest2, t0 =
startState)
35   stablePattern <- path[startStable:largeN]
36   empiricalStable <- rep(0, N+1)
37   for (i in stateNames) {
38     empiricalStable[i] <- mean( stablePattern ==
stateNames[i] )
39   }
40   theorStable <- steadyStates(ehrenfest2)
41   cat("Empirical stable distribution: ",
empiricalStable, "\n")
42   cat("Theoretical stable distribution: ",
theorStable, "\n")
43 }

```

R script for another alternative Ehrenfest Urn Model.

```

1  library(markovchain)
2
3  N <- 7; p <- 1/2; q <- 1 - p;
4  stateNames <- as.character( 0:N )
5  transMatrix <- matrix(0, N+1,N+1)
6  transMatrix[1,1] <- 1
7  transMatrix[N+1, N+1] <- 1
8  for (row in 2:N) {
9    transMatrix[row, row-1] <- ((N-(row-1))/N)*p
10   transMatrix[row,row] <- ((N-(row-1))/N)*q + ((row
-1)/N)*p
11   transMatrix[row,row+1] <- ((row-1)/N)*q
12 }
13 startState <- "3"
14
15 ehrenfest3 <- new("markovchain", transitionMatrix=
transMatrix,
16                 states=stateNames, name="Ehrenfest3"
)
17 print(ehrenfest3)
18
19 print( summary(ehrenfest3) )
20
21 pathLength <- 10
22 path <- rmarkovchain(n=pathLength,
23                     object = ehrenfest3, t0 =
startState)
24 cat("A sample starting from ", startState, path, "\n"
)

```

```

25 path <- rmarkovchain(n=pathLength,
26                       object = ehrenfest3, t0 =
27                         startState)
28 cat("Another sample starting from ", startState, path
29     , "\n")
30 if ( length( transientStates(ehrenfest3) ) == 0 ) {
31   largeN <- 1000; startStable <- 100
32   path <- rmarkovchain(n=largeN,
33                       object = ehrenfest3, t0 =
34                         startState)
35   stablePattern <- path[startStable:largeN]
36   empiricalStable <- rep(0, N+1)
37   for (i in stateNames) {
38     empiricalStable[i] <- mean( stablePattern ==
39                               i )
40   }
41   theorStable <- steadyStates(ehrenfest3)
42   cat("Empirical stable distribution: ",
43       empiricalStable, "\n")
44   cat("Theoretical stable distribution: ",
45       theorStable, "\n")
46 }

```

R script for yet another alternative Ehrenfest Urn Model.

```

1 library(markovchain)
2
3 N <- 7
4 stateNames <- as.character( 0:N )
5 transMatrix <- matrix(0, N+1,N+1)
6 transMatrix[1,1] <- 1
7 transMatrix[N+1, N+1] <- 1
8 for (row in 2:N) { #row 2 is state 1, row 7 is state
9   6
10   transMatrix[row, row-1] <- (row-1)*(N-(row-1))/N
11   ^2
12   transMatrix[row,row] <- (row-1)^2/N^2 + (N-(row
13   -1))^2/N^2
14   transMatrix[row,row+1] <- (row-1)*(N-(row-1))/N^2
15 }
16 startState <- "3"
17
18 ehrenfest4 <- new("markovchain", transitionMatrix=
19   transMatrix,
20   states=stateNames, name="Ehrenfest4"
21 )

```

```

17 print(ehrenfest4)
18
19 print( summary(ehrenfest4) )
20
21 pathLength <- 10
22 path <- rmarkovchain(n=pathLength,
23                     object = ehrenfest4, t0 =
24                     startState)
25 cat("A sample starting from ", startState, ":", path,
26     "\n")
27 path <- rmarkovchain(n=pathLength,
28                     object = ehrenfest4, t0 =
29                     startState)
30 cat("Another sample starting from ", startState, ":",
31     path, "\n")
32
33 if ( length( transientStates(ehrenfest4) ) == 0 ) {
34   largeN <- 1000; startStable <- 100
35   path <- rmarkovchain(n=largeN,
36                       object = ehrenfest4, t0 =
37                       startState)
38   stablePattern <- path[startStable:largeN]
39   empiricalStable <- rep(0, N+1)
40   for (i in seq_along(stateNames)) {
41     empiricalStable[i] <- mean( stablePattern ==
42                               stateNames[i] )
43   }
44   theorStable <- steadyStates(ehrenfest4)
45   cat("Empirical long-time distribution: ",
46       empiricalStable, "\n")
47   cat("Theoretical stable distribution: ",
48       theorStable, "\n")
49 }

```

#### 4.10. Problems to Work for Understanding

Chapter 4: Standard Examples.

- 4.1: For each of the urn models, express the transition probability  $P_{ij}$  of going to state  $j$  from state  $i$  in a general form, using the cases construction.
- 4.2: Prove that the stationary distribution for the first Ehrenfest Urn Model has entry  $\pi_i = \binom{k}{i}/2^k$ .
- 4.3: For the third and fourth Ehrenfest urn models with  $k = 7$  and  $p = q = 1/2$  which have absorbing states 0 and  $k$ , find the absorption probabilities and the expected waiting times to absorption from each transient state.

4.4: A certain system depends on a single machine that breaks down on any given day with probability  $p$ . It takes two days to restore the failed machine to normal service. Form a Markov chain by taking as states the pairs  $(x, y)$  where  $x$  is 1 if the machine is in operating condition at the end of a day, 0 otherwise and  $y$  is the number of days, 1 or 2 the machine has been broken. What is the long-term system availability?

4.5: Given  $m$  white balls and  $m$  black balls which are mixed thoroughly and then equally distributed in two urns,  $A$  and  $B$ . From each urn one ball is randomly drawn and placed in the other urn. Find the transition matrix and the probability that after a very large number of turns the first urn will have  $j$  white balls.

4.6: Unknown to public health officials, a person with a highly contagious disease enters the population. During each time period the person infects a new person with probability  $p$  or his symptoms appear and public health officials discover him, occurring with probability  $1 - p$  and quarantine him so that he is unable to infect additional people. Compute the probability distribution of the number of infected but undiscovered people in the population at the time of first discovery of a carrier. Assume each infected person behaves like the first.

## The Game of Monopoly as a Markov Chain

This chapter assumes familiarity with the standard layout and rules of the board game Monopoly, in particular, the classic U.S. version based on Atlantic City NJ with cards and rules in effect from 2008 to 2021. The goal is to model the game as a Markov chain to find the stationary distribution to determine the real estate squares a player token lands on most frequently. Those squares on the board are “more valuable” in the sense that other players will land on them more frequently and pay rent more frequently. Deciding which color group squares are “best” is more complicated because of the variable costs of rent and improvement costs around the board and that aspect is not considered here. The main intention of this chapter is to show how to successively make changes to a simple Markov chain to create a more nuanced model incorporating more transitions among states. Another intention is to analyze a Markov chain larger than introductory Markov chains.

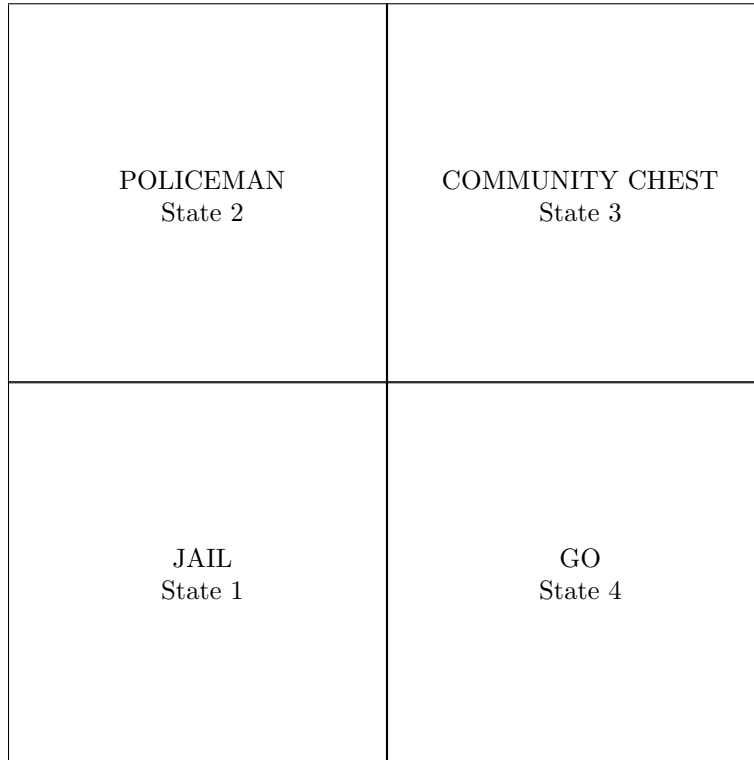
Student: contains scenes of mild algebra or calculus that may require guidance.

### 5.1. Chapter Starter Question

While playing the game of Monopoly, how often do you “take a walk on the Boardwalk”? That is, what is the fraction of time spent on the most expensive property in the game? How would you estimate this fraction?

### 5.2. A Simplified Four State Monopoly Game

The basic transition probability matrix around the Monopoly board is simply determined by the rolls of two fair six-sided dice. However making distant jumps due to the “Go To Jail” square and the drawing of certain *Community Chest* and *Chance* cards complicate the transition probability matrix. To understand this complication, first consider a much smaller example with just 4 spaces: Jail is state



**Figure 5.1.** A Monopoly board with 4 spaces.

1, Policeman is state 2, Community Chest is state 3, and Go is state 4, see Figure 5.1. A fair two-sided “die” (i.e. a fair coin) determines the 1 or 2 step forward motion of a player token around the board. Then the “dice roll” transition matrix  $R$  is

$$R = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{pmatrix}.$$

This transition probability matrix is regular, and that the stationary distribution is  $(1/4, 1/4, 1/4, 1/4)$ .

The “Jail” matrix represents the transition from landing on the Policeman:

$$J = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

This matrix differs from the identity matrix only in the second row (Policeman) where, with probability 1, a player goes directly to state 1, Jail.

The last element is the Community Chest state. Of the 16 Community Chest cards (including the Get Out of Jail Free card), 14 penalize or reward some peculiar accomplishment, e.g. \$10 for second prize in a beauty contest. However, one card sends the player to Jail, i.e. state 1, and the other card advances the player to Go, state 4. To form the Community Chest matrix, again start with the identity matrix and edit the third row to get

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{1}{16} & 0 & \frac{14}{16} & \frac{1}{16} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The transition matrix for the simplified 4-space board is then computed by the product

$$RJC = \begin{pmatrix} \frac{17}{32} & 0 & \frac{7}{16} & \frac{1}{32} \\ \frac{1}{32} & 0 & \frac{7}{16} & \frac{17}{32} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

The order of the factors reflects the process of the play: A player rolls first and then follows the actions of where the token lands, i.e. go to Jail, or draw a Community Chest card. Now the second row of the matrix gives the transition probabilities for a token on the Policeman's square. However, this square is never occupied, the second column of the product is entirely 0. Note that the conditional probabilities of going from Policeman state 2 to other states are not 0. In fact, those conditional probabilities are exactly what would be expected starting from square 2. But the probability of being at the Policeman state is 0, so these correctly calculated probabilities are irrelevant. In terms of Markov chain states, the Go, Jail, and Community Chest states are communicating and the Policeman state is not accessible from the other states. Deleting the second column and row from the matrix gives the transitions between the remaining 3 occupiable states. The stationary distribution is  $(\frac{16}{27}, \frac{7}{27}, \frac{4}{27})$ . The high frequency of landing in Jail in this truncated game is not surprising.

### 5.3. Full 40 State Monopoly Game

The states of the Markov chain representing the full game are the 40 spaces around the board, numbered 1 through 40 with Mediterranean Avenue as 1 and Go as 40.

The  $40 \times 40$  Rolling matrix has as its first row

$$[0, 0, \frac{1}{36}, \frac{2}{36}, \frac{3}{36}, \frac{4}{36}, \frac{5}{36}, \frac{6}{36}, \frac{5}{36}, \frac{4}{36}, \frac{3}{36}, \frac{2}{36}, \frac{1}{36}, 0, 0, \dots, 0].$$

The second row is a rotated version of this row, add a zero at the front and shift the nonzero entries one column to the right. Form each succeeding row the same way until eventually the first entry is nonzero, as the rolls start to wrap around the board. This creates a **circulant matrix**, a square matrix in which each row



vector is rotated one element to the right relative to the preceding row vector. Considering just this transition probability matrix, the steady state distribution is uniformly  $\frac{1}{40} = 0.025$  which is natural.

For now, continue to ignore the more complicated game rules about exiting from the Jail square, and let the  $J$  matrix be just the identity matrix with the 1 in row 30, Policeman, moved from column 30 to column 10, Jail.

The Community Chest spaces or states are 2, 17, and 33. Community Chest cards are most likely to give you money leaving the state unchanged. But two of the cards move the player either to Jail, state 10 or to Go, state 40. To form the Community Chest matrix  $Cc$ , change the 1 on the diagonal in row 30 of the identity matrix to  $\frac{14}{16}$  and enter  $\frac{1}{16}$  in each of column 10, Jail, and column 40, Go.

The Chance spaces or states are 7, 22 and 36. A Chance card is more likely than a Community Chest card to move players, 10 of the 16 cards directing a player to a different state. The existence of cards such as “Go back three spaces” and “Advance to the nearest railroad” means the transitions depend on which Chance a player lands on. The Chance matrix  $Ch$  differs from the identity in rows 7, 22 and 36. It makes sense to multiply the Community Chest matrix *after* the Chance matrix, since there is a probability  $\frac{1}{16}$  of moving from Chance state 36 to Community Chest state 33 and then to Go or Jail, each with probability  $\frac{1}{16}$ .

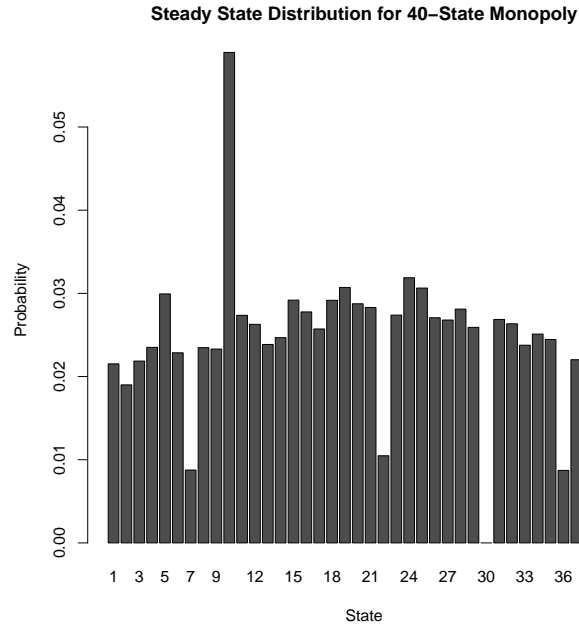
Finally, the full transition probability matrix is  $P = RJChCc$ . The stationary distribution gives a preliminary look at the proportion of time a player spends in each state over the course of a long game. The stationary distribution as a bar graph is in Figure 5.2. Table 5.1 summarizes the results with the 14 most frequently visited states in this model. The R script to generate the first two columns of Table 5.1 from the stationary distribution (eigenvector) of the transition probability matrix is in the Scripts section below. The last two columns come from a simulation with  $10^6$  steps. All states except 30 are communicating and the Policeman state 30 is not accessible from the other states. The frequencies computed here are essentially the same as the corresponding table in [AR97], with differences due to the number of significant digits reported.

#### 5.4. Modeling Rules for Jail

This first model and simulation ignores two finer aspects of the game. This model assumes a player sent to Jail immediately pays the \$50 fine or uses a Get Out of Jail card to exit Jail on the next roll. But late in a game, when the board is covered with hotels and houses with high rent, players may choose to stay in Jail for a couple of turns to avoid paying rents. The rules allow this for two turns unless doubles are rolled, in which case a player must leave, exposed to nearby high rents. Because one must leave Jail on the third roll, the model now needs a record of how many unsuccessful rolls of doubles have occurred. The solution is to define two new Jail states, one for being newly Jailed, now state 41 and the other for having failed at doubles exactly once, state 42. This is a small example of a general principle of turning a process which is not Markov into a Markov chain by adding states, for a general discussion, see [Str16]. The original Jail state 10 serves as both the

Rank	State	Frequency	Abbott	Abbott	Simulation	Simulation
			State	Frequency	State	
1	10	0.05896420	10	0.05896	10	0.058909
2	24	0.03187795	24	0.03188	24	0.031934
3	40	0.03113803	40	0.03114	40	0.031183
4	19	0.03071024	19	0.03071	19	0.030969
5	25	0.03063697	25	0.03064	25	0.030858
6	5	0.02993127	5	0.02993	5	0.029701
7	15	0.02918612	15	0.02919	15	0.029198
8	18	0.02916517	18	0.02917	18	0.029070
9	20	0.02874826	20	0.02875	20	0.028704
10	21	0.02830354	21	0.02830	28	0.028230
11	28	0.02810737	28	0.02811	21	0.028152
12	16	0.02776751	16	0.02777	16	0.028065
13	23	0.02738577	23	0.02739	23	0.027349
14	11	0.02735991	11	0.02736	11	0.027226

**Table 5.1.** The 14 most-frequently visited states in the simple 40-state model.



**Figure 5.2.** stationary distribution for the first 40-state model of Monopoly.

Rank	State	Frequency	Abbott	Abbott	Simulation	
			State	Frequency	State	Simulation
1	Jail	0.10799193	Jail	0.10800	Jail	0.108605
2	24	0.03012586	24	0.03013	24	0.030191
3	40	0.02948697	40	0.02949	40	0.029409
4	25	0.02905414	25	0.02905	25	0.029237
5	5	0.02845183	5	0.02845	19	0.028443
6	20	0.02821648	20	0.02822	5	0.028404
7	19	0.02821330	19	0.02821	20	0.028175
8	18	0.02811892	18	0.02812	18	0.028076
9	16	0.02674112	16	0.02674	28	0.026648
10	28	0.02669419	28	0.02669	16	0.026637
11	15	0.02658757	15	0.02659	15	0.026344
12	12	0.02636156	12	0.02636	12	0.026183
13	21	0.02627735	21	0.02628	21	0.026183
14	11	0.02602722	11	0.02603	11	0.026039

**Table 5.2.** The 14 most-frequently visited states in the 42 state model with Jail states 10, 41 and 42 combined.

Just-Visiting and twice-failed-rolling-doubles states, since in both cases, the player leaves on the next turn.

Table 5.2 gives the results of one simulation with  $10^6$  steps of this expanded Markov chain with the Jail states 10, 41 and 42 combined. State 10 now is a state reached by either a roll of the dice or by aging out of Jail so a player can move on to other states. The stationary distribution of this expanded Markov chain as a bar graph is in Figure 5.3, also with the Jail states 10, 41, and 42 combined.

The specific order of most frequently visited states is not as important as it appears in Table 5.2, since differences in frequency generally appear in the fourth significant digit. More useful is to consider *sets of most frequently visited states*. The most frequently visited set of states is 10, 41, 42, 24 and 40.

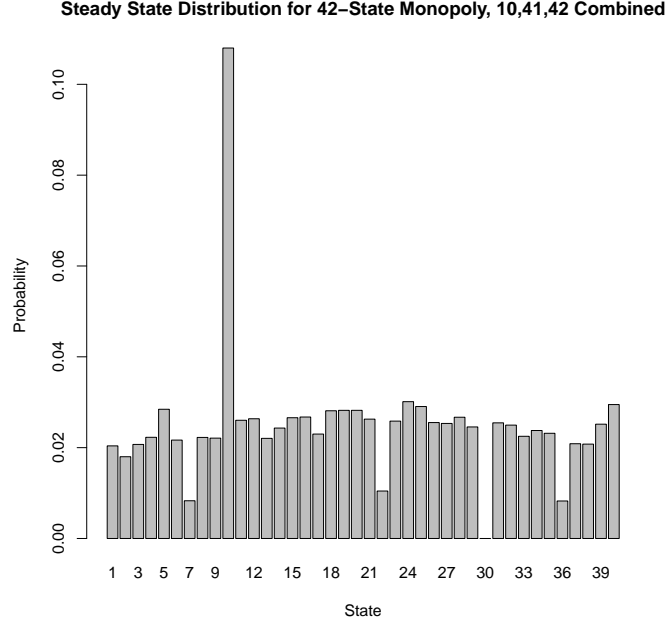
There is still one more detailed rule to consider, any player who rolls three doubles in a row goes to Jail. One way to handle this detail is to add 80 new states to the model as before, keeping track of history in a model with a total of 122 states. Again this illustrates the principle of turning a process which is not Markov into a Markov chain by adding states. An alternative way to handle this is to make an approximation by adjusting the Jail matrix  $J$  so that it sends a player not already in Jail to Jail with probability  $1/216$  since the probability of rolling three doubles in a row is  $\frac{1}{216}$ . Replace each 1 on the diagonal with  $\frac{215}{216}$  and add  $\frac{1}{216}$  to column 41. After making these last adjustments to the transition probability matrix, Table 5.3 summarizes the results of simulation. The stationary distribution for this final Markov chain model as a bar graph is in Figure 5.4.

---

Rank	State	Frequency
1	10	0.117841272
2	24	0.029795914
3	40	0.029055135
4	25	0.028235759
5	20	0.028148582
6	18	0.028019441
7	19	0.027108791
8	5	0.026894000
9	16	0.026694388
10	28	0.026549407
11	15	0.026091348
12	12	0.025963983
13	21	0.025481659
14	23	0.025471064
15	11	0.025384224
16	26	0.025192088
17	31	0.025076589
18	27	0.025064206
19	39	0.024766786
20	32	0.024499247
21	29	0.024398944
22	14	0.024354843
23	34	0.023334506
24	17	0.022984619
25	35	0.022713579
26	33	0.022086039
27	4	0.021986015
28	8	0.021786854
29	13	0.021756287
30	9	0.021606785
31	6	0.021335917
32	37	0.020478819
33	38	0.020476878
34	3	0.020438135
35	1	0.020087639
36	2	0.017758354
37	22	0.012115464
38	36	0.009514394
39	7	0.009452046
40	30	0.000000000

---

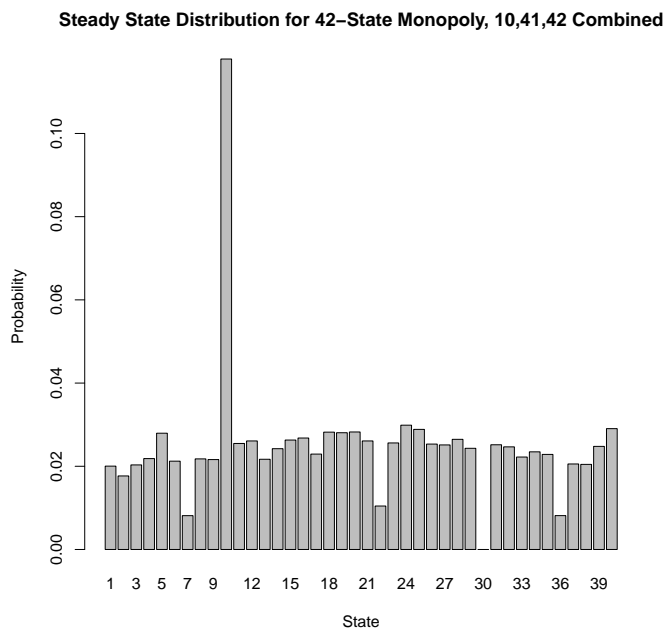
**Table 5.3.** The frequency of visited states in the final 42-state model with the approximation for going to Jail by rolling three doubles.



**Figure 5.3.** stationary distribution for the expanded 42-state model of Monopoly with Jail states 10, 41 and 42 combined.

### 5.5. Additional Modeling Considerations

A few modeling assumptions are not explicitly considered in this model. One assumption is that Community Chest and Chance card decks are shuffled after each draw so that drawing the cards is a random event, possibly even repeating. The game has 16 Community Chest cards including a “Get Out of Jail Free” card, which can be saved by the player who draws it. Assuming that card is in the deck and not retained gives the denominator of 16 used in the probabilities of the Community Chest matrix. Likewise, Monopoly uses 16 Chance cards but one is another “Get Out of Jail Free” card which can be saved. Assuming that card is still in the Chance deck gives the denominator of 16 used in the probabilities of the Chance matrix. This pair of assumptions makes equal denominators in the two matrices. Also, the final model assumes that appearance of a third consecutive roll of doubles is equally likely to occur at any space on the board, which is not strictly correct. Some squares are already known to be visited more than others and a third consecutive doubles could occur at an even number of squares further on the board from where the doubles run began. The refinements already made in modeling considerations are modifying the values of the stationary states by amounts on the order of  $10^{-3}$  or less. Since this is about the magnitude of the standard deviation of the frequency of visits in  $10^6$  steps, more precision cannot be realistically gained by refining the model.



**Figure 5.4.** stationary distribution for the final 42-state model of Monopoly.

In [AR97], Abbott and Richey use the stationary distribution to find the expected rental value and break-even times of the various color group properties. However, since illustration of the modeling and simulation of large Markov chains is the focus of these notes, these notes do not follow that investigation.

Many sites on the Internet make essentially the same Markov chain analysis of Monopoly in varying degrees of detail and in slightly different ways. For example, some use a 120-state chain to model the “rolling doubles” rule, and then condense the chain to the 40 board states. All reach essentially the same conclusions. Many of those sites go further and make an expected Return on Investment analysis to determine the most valuable spaces on the board, not just the most frequently visited. The Return on Investment analysis is not pursued here because the intention is to illustrate the Markov chain aspects.

## 5.6. Chapter Ending Answer

Since the board has 40 spaces, a first guess is that a token spends about  $1/40 = 0.025$  of the time on Boardwalk. In fact, using the most detailed Markov chain here, 0.02431 of the time is spent at Boardwalk. It is less than the easy estimate because the model shows that a much larger fraction of time is spent in Jail, and in fact, not all spaces are equally likely to be occupied.

## 5.7. Chapter Summary

### Key Concepts.

- (1) Modeling the game of Monopoly as a Markov chain finds the stationary distribution to find the properties landed on most frequently.
- (2) The modeling proceeds as a sequence of increasingly detailed Markov chains, each modeling more of the rules of the game.
- (3) The transition probability matrix is composed as a product of simpler transition matrices, each modeling a specific type of moves around the board.

### Vocabulary.

- (1) A **circulant matrix** is a square matrix in which each row vector is rotated one element to the right relative to the preceding row vector.

### Notation.

- (1)  $R$  – the “dice roll” transition probability matrix for the four state Monopoly
- (2)  $J$  – ‘Jail’ matrix represents the transition from landing on the Policeman
- (3)  $C$  – four state Community Chest matrix
- (4)  $Cc$  – full game Community Chest matrix
- (5)  $Ch$  – full game Chance matrix
- (6)  $P$  – full transition probability matrix

## 5.8. Sources

The section on Monopoly as a Markov chain is based on [AR97] with more information from [AB72]. Note that [AR97], uses the alternative convention that  $P_{ij}$  represents the probability of moving *to* state  $i$  *from* state  $j$ . Thus all matrices here are the transpose of matrices in [AR97]. Matthew Sheby pointed out an error in the Chance probability matrix in the scripts, now corrected so the stationary calculations agree with [AR97]. The simulation script is adapted from *Efficient R*, Chapter 7 by Colin Gillespie and Robin Lovelace.

## 5.9. Algorithms and Scripts

**Data:** States and basic transition probabilities

**Result:** stationary distribution for Monopoly game

```

1 function rotvec (v)
2   Cyclically rotate vector elements one place to right
3 return rotated vector

4 Initialization of Matrices
5 Load Markov Chain library
6 Set number of states and state names
7 Fill diceRoll matrix using rotvec
8 Fill diagonal Jail matrix with move from Police to Jail
9 Fill diagonal Community Chest matrix with moves to other states
10 Fill diagonal Chance matrix with moves to other states
11 Transition probability matrix as product of diceRoll, Jail, Chance and
    Community Chest
12 Markov chain calculations
13 Create Monopoly Markov chain object
14 Find stationary distribution of Monopoly Markov chain
15 return Selected results in table or graph

```

**Algorithm 6:** Monopoly Game Markov Chain



**Data:** Number of directly simulated Monopoly games  
**Result:** Empirical stationary distributions from simulations

```

1 function moveSquare (c, J)
2   Simulate roll of 2 dice and
3   keep track of jail time
4   return new state c and jail time J
5 function checkSquare (c)
6   Cyclically reduce state about state 40
7   return state number
8 function updateStateVector (c, J, l)
9   Keep track of number of times a state is visited
10  return updated landings l
11 function communityChest (c, J)
12  Move state according to random selection
13  of Community Chest card
14  return new state c and jail time J
15 function chance (c, J)
16  Move state according to random selection of Chance card
17  return new state c and jail time J
18 main mySimulateMonopoly (n)
19  Initialize landings vector to hold occupancy of states
20  Initialize jail time J
21  Initialize first state at Go
22  for i = 1 to numberOfTurns do
23    Move by moveSquare
24    if Chance square then
25      | move by chance
26    end
27    if Community Chest square then
28      | move by communityChest
29    end
30    Update landings
31  end
32  Set number of simulations n
33  Run mySimulateMonopoly n times, divide by n
34  return Relative Frequency of States from simulation

```

**Algorithm 7:** Simulation of Monopoly game

**R:** R script for 40-state Monopoly.

```

1 library("markovchain")
2
3 rotvec <- function(vec) vec[ c(length(vec), 1:(length
4                               (vec)-1)) ]

```

```

5 nStates <- 40
6 monopolyStates <- as.character( c(1:nStates) )
7
8 diceRoll <- matrix(0, nStates, nStates)
9 p1 <- c(0, 0,
10       1/36, 2/36, 3/36, 4/36, 5/36, 6/36, 5/36, 4/
11       36, 3/36, 2/36, 1/36,
12       numeric(nStates-13)
13       )
14 for (i in 1:nStates) {
15   diceRoll[i, ] <- p1
16   p1 <- rotvec(p1)
17 }
18 Jail <- diag(nStates)
19 Jail[30,30] <- 0
20 Jail[30, 10] <- 1
21
22 Ch <- diag(nStates)
23 chanceStates <- c(7, 22, 36)
24 chanceDests <- c(5, 10, 11, 24, 39, 40)
25 Ch[ cbind( chanceStates, chanceStates ) ] <- 7/16
26 Ch[ cbind( chanceStates, chanceStates-3 ) ] <- 1/16 #
27   Go Back 3 spaces
28 Ch[ chanceStates, chanceDests ] <- 1/16
29 Ch[7,12] <- 1/16; Ch[22,28] <- 1/16; Ch[36, 12] <- 1/
30   16 #nearest utility
31 Ch[7,15] <- 1/16; Ch[22,25] <- 1/16; #nearest
32   Railroad,
33 Ch[36, 5] <- 2/16 # note 2 ways to get to Reading
34   Railroad
35
36 Cc <- diag(nStates)
37 chestStates <- c(2, 17, 33)
38 chestDests <- c(10, 40)
39 Cc[ cbind(chestStates, chestStates) ] <- 14/16
40 Cc[chestStates, chestDests] <- 1/16
41
42 monopolyMatrix <- diceRoll %*% Jail %*% Ch %*% Cc
43
44 mcMonopoly <- new("markovchain", states =
45   monopolyStates, byrow = TRUE,
46   transitionMatrix = monopolyMatrix,
47   name = "Monopoly")
48 ss <- steadyStates(mcMonopoly)
49

```

```

44 top14ofAbbott <- (1/100)*c(5.896, 3.188, 3.114,
    3.071, 3.064, 2.993, 2.919, 2.917, 2.875, 2.830,
    2.811, 2.777, 2.739, 2.736)
45 top14ofAbbottIndices <- c(10, 24, 40, 19, 25, 5, 15,
    18, 20, 21, 28, 16, 23, 11)
46
47 sstop14 <- sort(ss, decreasing=TRUE)[1:14]
48 sstop14Indices <- order(ss, decreasing=TRUE)[1:14]
49
50 maxDiff <- max( abs( sstop14 - top14ofAbbott) )
51 cat("Maximum Difference: ", maxDiff, "\n")
52 maxDiffIndex <- which.max( abs( sstop14 -
    top14ofAbbott) )
53 cat("Maximum Difference Index: ", maxDiffIndex, "\n")
54 maxRelDiff <- maxDiff/sstop14[maxDiffIndex]
55 cat("Relative Maximum Difference: ", maxRelDiff, "\n"
    )
56
57 ssdf <- data.frame( sstop14Indices, sstop14)
58
59 barplot(ss, names.arg=1:40,
60     main="Steady State Distribution for 40-State
    Monopoly",
61     xlab="State", ylab="Probability")

```

R script for 42-state Monopoly.

```

1  library("markovchain")
2
3  rotvec <- function(vec) vec[ c(length(vec), 1:(length
    (vec)-1)) ]
4
5  nStates <- 42
6  monopolyStates <- as.character( c(1:nStates) )
7
8  diceRoll <- matrix(0, (nStates-2), (nStates-2))
9  p1 <- c(0, 0,
10     1/36, 2/36, 3/36, 4/36, 5/36, 6/36, 5/36,
    4/36, 3/36, 2/36, 1/36,
11     numeric((nStates-2)-13)
12     )
13 for (i in 1:(nStates-2)) {
14     states 1 through 40
15     diceRoll[i, ] <- p1
16     p1 <- rotvec(p1)
17 }

```

```

17 ## Next, no probability of going from board state to
    extra Jail states
18 diceRoll <- cbind(diceRoll, matrix(0, (nStates-2),
    2))
19 ## add rows from extra Jail states
20 diceRoll <- rbind(diceRoll, matrix(0, 2, nStates))
21 ## fill transitions for rolling doubles to get out of
    Jail
22 diceRoll[41, 41] <- 0; diceRoll[41, 42] <- 5/6 #stay
    in jail one turn
23 diceRoll[41, c(12, 14, 16, 18, 20, 22)] <- 1/36 #roll
    doubles
24 diceRoll[42, 42] <- 0; diceRoll[42, 10] <- 5/6 #stay
    in Jail one more turn
25 diceRoll[42, c(12, 14, 16, 18, 20, 22)] <- 1/36 #roll
    doubles
26
27 Jail <- diag(nStates)
28 Jail[30,30] <- 0
29 Jail[30, 41] <- 1 #go from
    Police to Jail
30
31 Cc <- diag(nStates)
32 chestStates <- c(2, 17, 33)
33 chestDests <- c(40, 41)
34 Cc[ cbind(chestStates, chestStates) ] <- 14/16
35 Cc[chestStates, chestDests] <- 1/16
36
37 Ch <- diag(nStates)
38 chanceStates <- c(7, 22, 36)
39 chanceDests <- c(5, 11, 24, 39, 40, 41)
40 Ch[ cbind( chanceStates, chanceStates ) ] <- 7/16
41 Ch[ cbind( chanceStates, chanceStates-3 ) ] <- 1/16 #
    Go Back 3 spaces
42 Ch[ chanceStates, chanceDests] <- 1/16
43 Ch[7,12] <- 1/16; Ch[22,28] <- 1/16; Ch[36, 12] <-
    1/16 #nearest utility
44 Ch[7,15] <- 1/16; Ch[22,25] <- 1/16; #nearest
    Railroad,
45 Ch[36, 5] <- 2/16 # note 2 ways to get to Reading
    Railroad
46
47 monopMat <- diceRoll %*% Jail %*% Ch %*% Cc
48
49 mcMonopoly42 <- new("markovchain", states =
    monopolyStates, byrow = TRUE,

```

```

50 transitionMatrix = monopMat, name =
    "Monopoly")
51 ss <- steadyStates(mcMonopoly42)
52
53 ssComb <- ss
54 ssComb[10] <- ssComb[10] + ssComb[41] + ssComb[42]
55 ssCombTop14 <- sort(ssComb[1:40], decreasing=TRUE)
    [1:14]
56 ssCombTop14Indices <- order(ssComb[1:40], decreasing=
    TRUE)[1:14]
57 ssCombdF <- data.frame( ssCombTop14Indices,
    ssCombTop14)
58
59 top14ofAbbott <- (1/100)*c(10.800, 3.013, 2.949,
    2.905, 2.845, 2.822, 2.821, 2.674, 2.669, 2.659,
    2.659, 2.636, 2.628, 2.603)
60 top14ofAbbottIndices <- c(10, 24, 40, 25, 5, 20, 19,
    18, 16, 28, 15, 12, 21 , 11)
61
62 maxDiff <- max( abs( ssCombTop14 - top14ofAbbott) )
63 cat("Maximum Difference: ", maxDiff, "\n")
64 maxDiffIndex <- which.max( abs( ssCombTop14 -
    top14ofAbbott) )
65 cat("Maximum Difference Index: ", maxDiffIndex, "\n")
66 maxRelDiff <- maxDiff/ssCombTop14[maxDiffIndex]
67 cat("Relative Maximum Difference: ", maxRelDiff, "\n"
    )
68
69 barplot(ssComb[1:40], names.arg=1:40,
70     main="Steady State Distribution for 42-State
    Monopoly, 10,41,42 Combined",
71     xlab="State", ylab="Probability")

```

R script to simulate 42-state Monopoly.

```

1  ## This function calculates where you will land on
    your next move.
2  moveSquare <- function(current, jailTime) {
3      dice <- sample(seq(1,6), 2, replace=TRUE)
4
5      if (current == 10 & jailTime > 0) { # in Jail
6          if (dice[1] == dice[2]) {      # roll
7              doubles!
8              current <- 10 + sum(dice)    # get out
9              of Jail
10             jailTime <- 0

```

```

9         } else {                                     #don't
move but...
10         jailTime <- (jailTime + 1) %% 3 # count
up jail time
11     }
12     } else {
13         current <- current + sum(dice)             # regular
roll
14     }
15     return(c(current, jailTime))
16 }
17
18 ## Helper function to avoid code replication
19 checkState <- function(current) {
20     if (current > 40) {
21         current <- current - 40
22     } else if (current < 1) {
23         current <- current + 40
24     }
25     return(current)
26 }
27
28 ## Helper function to record landings,
29 updateStateVector <- function(current, jailTime,
landings) {
30     if (current == 10 & jailTime > 0) {
31         landings[40 + jailTime] = landings[40 +
jailTime] + 1
32     } else {
33         landings[current] <- landings[current] + 1
34     }
35
36     return(landings)
37 }
38
39 ## Move according to community chest cards
40 ## Use 16 cards, Get Out of Jail is reserved
41 communityChest <- function(current, jailTime) {
42     u <- runif(1)
43     goto <- current # Default. Do nothing
44     if (u < 1 / 16) {
45         goto <- 40 # Go
46     } else if (u < 2 / 16) {
47         goto <- 10 # Jail
48         jailTime <- 1
49     }
50     return( c(goto, jailTime) )

```

```

51 }
52
53 ## Move according to chance cards
54 ## Use 16 cards, Get Out of Jail is NOT reserved
55 chance <- function(current, jailTime) {
56   u <- runif(1)
57   goto <- current # Default. Do nothing
58   if (u < 1 / 16) {
59     goto <- 40 # Go
60   } else if (u < 2 / 16) {
61     goto <- 24 # Illinois Ave.
62   } else if (u < 3 / 16) {
63     goto <- 11 # St. Charles Place
64   } else if (u < 4 / 16) {
65     goto <- 10 # Jail
66     jailTime <- 1
67   } else if (u < 5 / 16) {
68     goto <- 5 # Take ride on Reading
69   } else if (u < 6 / 16) {
70     goto <- 39 # Boardwalk
71   } else if (u < 7 / 16) {
72     goto <- checkState(current - 3) # Must check,
73     since goto maybe negative!
74   } else if (u < 8 / 16) {
75     if (current > 28 | current < 12) { # Advance
76       to nearest Utility
77       goto <- 12 # Water Works
78     } else {
79       goto <- 28 # Electricity
80     }
81   } else if (u < 9 / 16) { # Advance to nearest
82     Railroad
83     if (current > 35 | current < 5) {
84       goto <- 5 # Reading
85     } else if (current > 5 & current < 15) {
86       goto <- 15 # Pennsylvania
87     } else if (current > 15 & current < 25) {
88       goto <- 25 # B & O
89     } else if (current > 25 & current < 35) {
90       goto <- 35 # Short Line
91     }
92   }
93   return(c(goto, jailTime))
94 }
95
96 ## Main, record where landings occur
97 mySimulateMonopoly <- function (numberOfTurns)

```

```

95 {
96   landings <- numeric(42) # vector to hold
occupancy of states,
97   # 1 is Med Ave, 40 is Go
98   # 41 is in Jail for one turn, 42 is Jail for two
turns
99   # 10 is Just Visiting Jail or Jail for three
turns, ready to get out
100   jailTime <- 0
101   current <- 40 # start at Go
102   for (i in 1:numberOfTurns) {
103     moveState <- moveSquare(current, jailTime)
104     current <- moveState[1]
105     jailTime <- moveState[2]
106     current <- checkState(current)
107     if (current == 30) {
108       current <- 10
109       jailTime <- 1
110     }
111     if (current == 7 | current == 22 | current ==
36) {
112       move <- chance(current, jailTime)
113       current <- move[1]
114       jailTime <- move[2]
115     }
116     if (current == 2 | current == 17 | current ==
33) {
117       move <- communityChest(current, jailTime)
118       current <- move[1]
119       jailTime <- move[2]
120     }
121     landings <- updateStateVector(current,
jailTime, landings) # must do update
122   }
123   return(landings)
124 }
125
126 n <- 1000
127 ss <- mySimulateMonopoly(n)/n

```

## 5.10. Problems to Work for Understanding

Chapter 5: The Game of Monopoly as a Markov Chain.

5.1: Create a small Monopoly game with just 8 spaces:

(1) Reading Railroad is state 1,



- (2) Jail is state 2,
- (3) Pennsylvania Railroad is state 3,
- (4) Policeman is state 4,
- (5) B. & O. Railroad is state 5,
- (6) Chance is state 6,
- (7) Short Line is state 7 and
- (8) Go is state 8.

A fair two-sided “die” (i.e. a fair coin) determines the 1 or 2 step forward motion of a player token around the board. Considering this as a Markov Chain, find the stationary distribution. Assume the simple rule that a player leaves Jail immediately, no staying for 2 more turns. Be sure to include the effect drawing an “Advance to the Nearest Railroad”, “Take a Ride on the Reading”, “Go to Jail”, “Advance to Go”, or “Go back 3 spaces” card from the Chance deck. All other Chance movement cards (e.g. Illinois Avenue, Boardwalk, Utility) have no effect on movement.

# The Game of Risk as a Markov Chain

This chapter uses Markov chains to analyze the stochastic progress of a war between two players in the board game *Risk*. Standard Markov chain methods give the probabilities of victory and additionally the expected losses in a war.

Mathematically Mature: contains mathematics beyond calculus with proofs.

## 6.1. Chapter Starter Question

When rolling three fair six-sided dice with outcomes  $Y_1, Y_2, Y_3$ , what are the order statistics of the outcome?

## 6.2. The Game of Risk

The board game *Risk* for two or more players has a world map separated into 42 territories. Each player has a number of tokens used as armies. Each token represents one army. A player may use some or all but one of the armies to attack the armies in an adjacent opponent-controlled territory. The goal of a player is either to conquer the world through wars or to fulfill a task assigned at the beginning of the game. This task can be destroying a specific enemy or conquering a specific area.

The game consists of wars between two players, and each war consists of one or more rounds of combat. At each turn, a player must decide whether or not to attack a territory. The first question is the following: *If a player attacks a territory with some armies, what is the probability the player will capture this territory?* Of course, the probability that a player will capture a territory could be high while the expected loss is also high. Therefore, the second question is: *If a player engages in a war, how many armies should the player expect to keep, depending on the number of armies the opponent has on that territory?*

Case	Number of Armies		Number of Dice	
	Attacker	Defender	Attacker	Defender
1	1	1	1	1
2	2	1	2	1
3	$\geq 3$	1	3	1
4	1	$\geq 2$	1	2
5	2	$\geq 2$	2	2
6	$\geq 3$	$\geq 2$	3	2

**Table 6.1.** The number of dice each player rolls according to the number of attacker and defender armies.

At each turn, a player occupying some region may attack a neighboring territory. An attacker must leave at least one army on the occupied territory, and use at least one army in an attack. Thus a player who has at least two armies (one to keep on the territory and one to attack a territory) may attack a neighbor territory. A player who decides to attack a territory declares war on the opponent and the two players engage in a sequence of combats with random outcomes determined by dice. Outcomes of the defender's and the attacker's dice decide each battle and the ultimate outcome of the war. An attacker may withdraw before the war ends. An attacker who does not withdraw either destroys all the defender armies in that territory and occupies that territory, or loses all the attacking armies and fails to conquer the territory.

The number of armies an attacker or a defender possesses at the start of a each battle determines the number of dice each player rolls. To begin a round of war, the attacker will roll one die if attacking with a single army, two dice if the attacker has two armies present, and three dice if the attacking player has three or more armies involved in the war. A defender rolls one die with one army and two dice with two or more armies in the embattled territory. Six different cases result from the number of dice each opponent rolls, see Table 6.1.

At each turn, after rolling the dice, each player sets the dice in descending order and then pairs off the two sets of dice, matching the highest attacking die roll against the highest defending die roll. If each player is using at least two dice, then the second highest die rolls are similarly matched. The attacker loses one army for each die that is less than or equal to the corresponding defender's die. The defender loses one army for each die that is strictly less than the corresponding attacker's die. Note that ties favor the defender, so each tie results in the loss of an attacking army. After taking away the armies lost at that turn, the players roll the dice again. This sequence continues until one side loses all of its armies. Table 6.2 shows the progress of a typical war for a country. This war took four battles. At the end of the fourth turn, the attacker lost all of the attacking armies and the defender wins the war. This table also serves as a reminder of the number of dice rolled in various situations, never more than three for the attacker, and never more than two for the defender.

It may be disadvantageous to take control of a new territory by winning a war with only one army remaining, emphasizing the importance of the second question:

Roll	Armies		Dice Rolled		Dice Outcome		Losses	
	Att	Def	Att	Def	Att	Def	Att	Def
1	4	3	3	2	5,4,3	6,3	1	1
2	3	2	3	2	5,5,3	5,5	2	0
3	1	2	1	2	6	4,3	0	1
4	1	1	1	1	5	6	1	0
5	0	1						

**Table 6.2.** An example of a war with 4 battles

*If a player engages in a war, how many armies should the player expect to lose depending on the number of armies the opponent has on that territory?*

### 6.3. Risk States

Let  $A$  be the number of attacking armies and  $D$  the number of defending armies. The values of  $A$  and  $D$  characterize the state of the system at a given time. Let  $X_n$  be the state of the system at the beginning of the  $n$ th turn:

$$X_n = (a_n, d_n), \quad 0 \leq a_n \leq A, 0 \leq d_n \leq D$$

where  $a_n$  and  $d_n$  are the number of attacking and defending armies respectively. The initial state of the system is  $X_0 = (A, D)$ . If one side loses all its armies then that side loses the war; i.e., if  $X_n = (0, d_n)$  with  $d_n > 0$ , then the attacker has lost the war at the end of the turn. Similarly, if  $X_n = (a_n, 0)$ , with  $a_n > 0$ , then the attacker has won the war at the end of the turn. Given the number of armies each side has at a given round, then it is possible to calculate the probability that each side wins or loses the war without knowing the states of the system before that round. In other words, the war process has the Markov property.

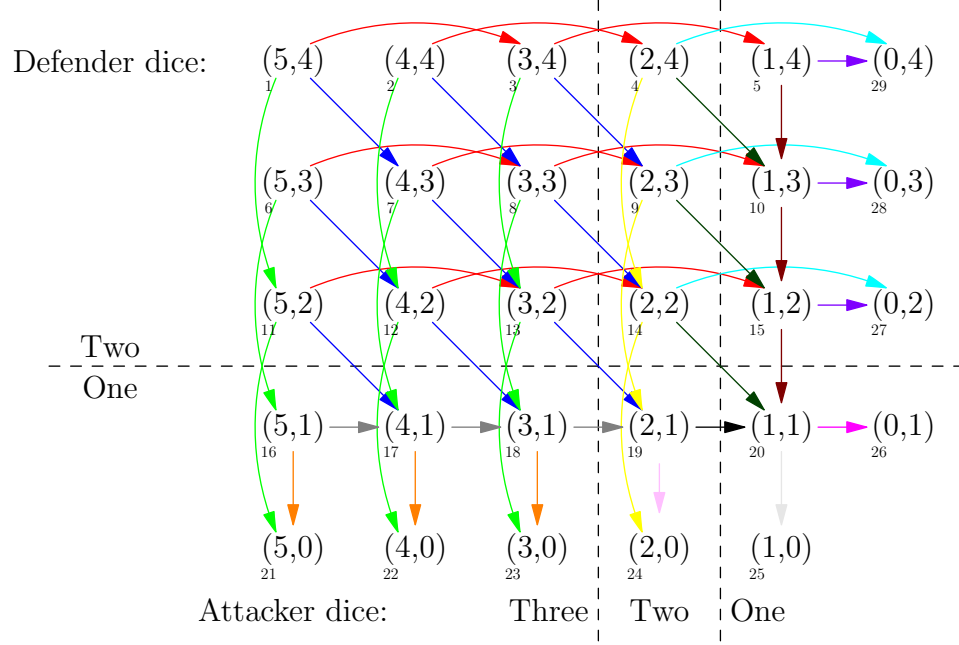
The  $AD$  states with both  $a$  and  $d$  positive are transient. The  $A+D$  states where either  $a = 0$  or  $d = 0$  are absorbing. Order the  $AD + A + D$  possible states so that the  $AD$  transient states precede the  $A + D$  absorbing states. Order the transient states with the attacker armies decreasing along a row for constant defenders, and the defender armies decreasing row by row, see Figure 6.1. The transient states are, in order

$$\begin{aligned} &(A, D), (A-1, D), (A-2, D), \dots, (1, D), \\ &(A, D-1), (A-1, D-1), \dots, (1, D-1), \\ &\dots \\ &(A, 1), (A-1, 1), \dots, (1, 1). \end{aligned}$$

Order the absorbing states by decreasing desirability of outcome for the attacker, including the absorbing states where the defender wins

$$(A, 0), (A-1, 0), \dots, (1, 0), (0, 1), (0, 2), \dots, (0, D).$$

Note that this order is the reverse of the state order in [Os03]. The order here proceeds in the general direction of the war, with the first state for the initial numbers of armies, then decreasing number of armies for both players. See Figure 6.1



**Figure 6.1.** The state space and transitions of the Markov chain for a war in *Risk*. Transitions of the same color have the same probability.

for a diagram of the possible state transitions when  $A = 5$  and  $D = 4$ . This figure is key for understanding the Markov chain. The small number below each ordered pair state is the index of the state for the transition probability matrix. The state indices increase from left to right and top to bottom, so the state of the system flows from the upper left corner to the bottom or right margin. The diagram divides into 6 regions, 3 for the attacker, and 2 for the defender depending on the number of dice each is rolling in a battle, as already outlined in Table 6.1. For example, the lower right region corresponds to Case 1 in Table 6.1 and the transition probabilities  $\rho_{111}$  and  $\rho_{110}$  detailed below in Table 6.3. The largest region in the upper left corresponds to Case 6 in Table 6.1 and the transition probabilities  $\rho_{32\ell}$  in Table 6.3. Likewise for the other regions. Figure 6.1 labels the possible state transitions with arrows and colors corresponding to the transition probabilities in Table 6.3.

The states and the coordinates of states on the diagram can be confusing. For instance, the initial armies state  $(5, 4)$  is at location  $(x = 1, y = 4)$  on the diagram. As the attacking armies decrease, the first coordinate of the location of the state increases. As the defending armies decrease, the second coordinate of the location decreases. This means:

- writing computer code for the chart requires close attention to indices, and
- do not confuse location with state.

### 6.4. Transition Probabilities

Under this ordering, the transition probability matrix takes the block-matrix form

$$P = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix}$$

where the  $(AD) \times (AD)$  matrix  $Q$  has the probabilities of going from one transient state to another, and the  $(AD) \times (A+D)$  matrix  $R$  has the probabilities of going from a transient state into an absorbing state. Note that this is the opposite order than the order in the chapter on Waiting Time to Absorption. The transition probability matrix  $P$  contains only 14 distinct probability values, based on the number of dice rolled and the armies lost as a result. Let  $\rho_{ij\ell}$  denote the probability that the defender loses  $\ell$  armies when rolling  $j$  dice against an attacker rolling  $i$  dice. See Table 6.3. To calculate  $\rho_{ij\ell}$ , find the joint probabilities associated with the best and second best roll from 2 or 3 six-sided fair dice. Let  $Y_1, Y_2, Y_3$  denote the unordered outcome for an attacker when rolling three dice and let  $W_1, W_2$  denote the unordered outcome for an attacker when rolling two dice. Let  $Z_1, Z_2$  denote the unordered outcome for a defender rolling two dice. Then  $Y_1, Y_2, Y_3, W_1, W_2$  and  $Z_1, Z_2$  are random samples from the discrete uniform distribution on the integers 1 through 6. For example,

$$\mathbb{P}[Y_j = y] = \begin{cases} \frac{1}{6} & \text{if } y = 1, 2, 3, 4, 5, 6, \\ 0 & \text{else.} \end{cases}$$

Given a sample of  $n$  identically distributed random values, the  $\ell$ th **order statistic** is the  $\ell$ th largest value. Using superscripts, the ordered random variables  $Y^{(1)} \geq Y^{(2)} \geq Y^{(3)}$  are the order statistics for the 3-dice attacker roll, the ordered random variables  $W^{(1)} \geq W^{(2)}$  are the order statistics for the 2-dice attacker roll, and the ordered random variables  $Z^{(1)} \geq Z^{(2)}$  are the order statistics for the 2-dice defender roll. The joint distributions of the order statistics for specification of  $\rho_{ij\ell}$  use straightforward techniques of enumeration. When rolling two dice, the joint distribution of  $(Z^{(1)}, Z^{(2)})$  is

$$\mathbb{P}[Z^{(1)} = z^{(1)}, Z^{(2)} = z^{(2)}] = \begin{cases} \frac{1}{36}, & \text{if } z^{(1)} = z^{(2)} \\ \frac{2}{36}, & \text{if } z^{(1)} > z^{(2)} \\ 0, & \text{else.} \end{cases}$$

See Figure 6.2 for the probability of  $Z^{(1)} = 5, Z^{(2)} = 3$ . The *marginal distribution* of the best roll  $Z^{(1)}$  sums the joint distribution over possible values of  $z^{(2)} \leq z^{(1)}$ :

$$\mathbb{P}[Z^{(1)} = z^{(1)}] = \frac{2z^{(1)} - 1}{36}$$

for  $z^{(1)} = 1, 2, 3, 4, 5, 6$ . See Figure 6.3 for the probability of  $Z^{(1)} = 5$ . When rolling three dice, the distribution of the best two rolls is

$$\mathbb{P}[Y^{(1)} = y^{(1)}, Y^{(2)} = y^{(2)}] = \begin{cases} \frac{3y^{(1)} - 2}{216}, & \text{if } y^{(1)} = y^{(2)}, \\ \frac{6y^{(2)} - 3}{216}, & \text{if } y^{(1)} > y^{(2)}, \\ 0, & \text{else.} \end{cases}$$

	1	2	3	4	5	6
1						
2						
3					$\frac{1}{36}$	
4						
5			$\frac{1}{36}$			
6						

**Figure 6.2.** Visualization of  $Z^{(1)} = 5$ ,  $Z^{(2)} = 3$ .

	1	2	3	4	5	6
1	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
2	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
3	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
4	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
5	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
6	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$

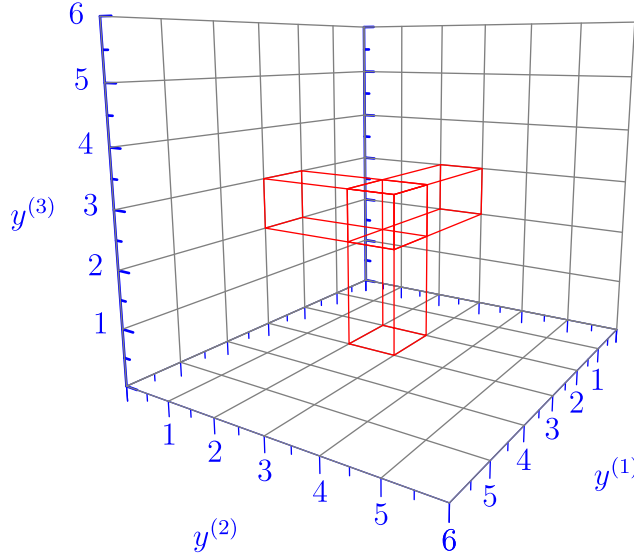
**Figure 6.3.** Visualization of  $Z^{(1)} = 5$ .

See Figure 6.4 for the probability of  $Y^{(1)} = 3$ ,  $Y^{(2)} = 3$ . See the exercises for the derivation of the entry for  $Y^{(1)} = y^{(1)}$ ,  $Y^{(2)} = y^{(2)}$  with  $y^{(1)} > y^{(2)}$ . The marginal distribution of the best roll is

$$\mathbb{P} \left[ Y^{(1)} = y^{(1)} \right] = \frac{1 - 3y^{(1)} + 3(y^{(1)})^2}{216}$$

for  $y^{(1)} = 1, 2, 3, 4, 5, 6$ . All of the probabilities are 0 for arguments that are not positive integers less than or equal to 6. The joint distribution of  $W^{(1)}$  and  $W^{(2)}$  is the same as that for  $Z^{(1)}$  and  $Z^{(2)}$ .

Now it is possible to calculate specific transition probabilities using these marginal distributions. Let  $\rho_{ij\ell}$  be the probability the attacker rolls  $i$  dice, the defender



**Figure 6.4.** Visualization of  $Y^{(1)} = 3, Y^{(2)} = 3$ .

rolls  $j$  dice and the defender loses  $\ell$  armies. For example

$$\begin{aligned}
 \rho_{322} &= \mathbb{P} \left[ Y^{(1)} > Z^{(1)}, Y^{(2)} > Z^{(2)} \right] \\
 &= \sum_{z_1=1}^5 \sum_{z_2=1}^{z_1} \mathbb{P} \left[ Y^{(1)} > z_1, Y^{(2)} > z_2 \right] \mathbb{P} \left[ Z^{(1)} = z_1, Z^{(2)} = z_2 \right] \\
 &= \sum_{z_1=1}^5 \sum_{z_2=1}^{z_1} \sum_{y_1=z_1+1}^6 \sum_{y_2=z_2+1}^{y_1} \mathbb{P} \left[ Y^{(1)} = y_1, Y^{(2)} = y_2 \right] \mathbb{P} \left[ Z^{(1)} = z_1, Z^{(2)} = z_2 \right] \\
 &= \frac{2890}{7776} \\
 &\approx 0.372
 \end{aligned}$$

Note that those events in this quadruple sum for which an argument with a subscript of 2 exceeds an argument with the same letter and subscript 1 have probability zero.

Each entry of the transition probability matrix  $P$  is one of the 14 values  $\rho_{ij\ell}$  according to the arrows in Figure 6.1 or the outcomes in Table 6.3. The exact probabilities and the decimal approximation rounded to 3 places, are in Table 6.3. The colors refer to the colors of the arrows representing transitions in Figure 6.1.

## 6.5. Absorption Probabilities

Given any initial state, the system *eventually* makes a transition to an absorbing state. For a transient state  $i$ , call  $f_{ij}^{(n)}$  the probability that the first (and final) visit to absorbing state  $j$  occurs on the  $n$ th turn:

$$f_{ij}^{(n)} = \mathbb{P} [X_n = j, X_\nu \neq j \text{ for } \nu = 1, 2, \dots, n-1 \mid X_0 = i].$$



Att Dice	Def Dice	Outcome	Symbol	Exact Prob.	Approx. Prob.	Color
1	1	Def loses 1	$\rho_{111}$	15/36	0.417	light gray
1	1	Att loses 1	$\rho_{110}$	21/36	0.583	magenta
1	2	Def loses 1	$\rho_{121}$	55/216	0.255	brown
1	2	Att loses 1	$\rho_{120}$	161/216	0.745	purple
2	1	Def loses 1	$\rho_{211}$	125/216	0.579	pink
2	1	Att loses 1	$\rho_{210}$	91/216	0.421	black
2	2	Def loses 2	$\rho_{222}$	295/1296	0.228	cyan
2	2	Each lose 1	$\rho_{221}$	420/1296	0.324	darkgreen
2	2	Att loses 2	$\rho_{220}$	581/1296	0.448	yellow
3	1	Def loses 1	$\rho_{311}$	855/1296	0.660	orange
3	1	Att loses 1	$\rho_{310}$	441/1296	0.340	gray
3	2	Def loses 2	$\rho_{322}$	2890/7776	0.372	green
3	2	Each lose 1	$\rho_{321}$	2611/7776	0.336	blue
3	2	Att loses 2	$\rho_{320}$	2275/7776	0.293	red

**Table 6.3.** Probabilities in the transition probability matrix. The colors correspond to the arrows in the diagram of state transitions.

Denote the  $AD \times (A+D)$  matrix of these first transition probabilities by  $F^{(n)}$ . Then  $F^{(n)} = Q^{n-1}R$ . The probability that the system eventually goes from transient state  $i$  to absorbing state  $j$  is  $F = (I - Q)^{-1}R$ . If the system ends in one of the  $A$  absorbing states then the attacker wins; if it ends in one of the  $D$  absorbing states, the defender wins. Since the initial state of a war is the first state using the order established previously, the probability that the attacker wins is just the sum of the entries in the first row of the submatrix of the first  $A$  columns of  $F$ :

$$\mathbb{P}[\text{Attacker wins} \mid X_0 = (A, D)] = \sum_{j=1}^A f_{1,j}$$

and

$$\mathbb{P}[\text{Defender wins} \mid X_0 = (A, D)] = \sum_{j=A+1}^{A+D} f_{1,j}.$$

Because the state order here is the reverse of the order given in [Os03], the table of winning probabilities here is the reverse of Table 3 in that paper. Note also by the Markov property, by calculating the winning probability for say  $A = 10$  and  $D = 10$ , the winning probability for any war starting with  $A < 10$  and  $D < 10$  is also automatically calculated so that the entire Table 6.4 comes from  $F = (I - Q)^{-1}R$  for  $A = 10$  and  $D = 10$ .

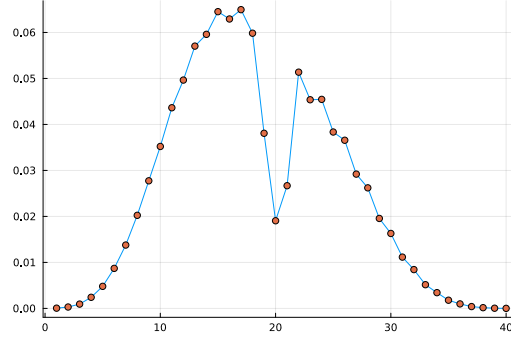
Att Def	10	9	8	7	6	5	4	3	2	1
10	0.568	0.480	0.380	0.287	0.193	0.118	0.057	0.021	0.001	0.000
9	0.650	0.558	0.464	0.357	0.258	0.162	0.086	0.033	0.003	0.000
8	0.724	0.646	0.547	0.446	0.329	0.224	0.123	0.054	0.005	0.000
7	0.800	0.726	0.643	0.536	0.423	0.297	0.181	0.084	0.011	0.000
6	0.861	0.808	0.730	0.640	0.521	0.397	0.253	0.134	0.021	0.000
5	0.916	0.873	0.818	0.736	0.638	0.506	0.359	0.206	0.049	0.002
4	0.954	0.930	0.888	0.834	0.745	0.638	0.477	0.315	0.091	0.007
3	0.981	0.967	0.947	0.910	0.857	0.769	0.642	0.470	0.206	0.027
2	0.994	0.990	0.980	0.967	0.934	0.890	0.785	0.656	0.363	0.106
1	1.000	1.000	1.000	0.999	0.997	0.990	0.972	0.916	0.754	0.417

**Table 6.4.** Probability that the attacker wins with  $A$  armies against  $D$  defending armies.

Large engagements occur towards the end of an entire game of *Risk*. The absorbing probabilities for large wars have an interesting “saw-tooth” feature first noticed in [PW15]. Figure 6.5 shows the probability mass function when the attacker and defender each start with 20 armies. The horizontal axis shows all the absorbing states of a (20, 20) war and the vertical axis is the probability of the corresponding absorbing state. The outcome states along the horizontal axis are in decreasing order of preference of the attacker. One distinctive feature of this probability mass function is the local minimum at 20 in the probability masses. The outcomes (1, 0) and (0, 1) are less likely than their neighbors (2, 0) and (0, 2). The outcomes (2, 0) and (0, 2) can occur when a player with a single army will roll only one die against two dice and is less likely to survive. Also interesting is the jagged or “saw-tooth” phenomenon near the local maxima. A final outcome of (4, 0) or (6, 0) is each more likely than an outcome of (5, 0). In the largest part of the transient states the probability of removing *two* armies from one player is about double the probability of each player losing *one* army. So a path that begins with both armies with the same parity is more likely to visit only states  $(a, d)$  in which  $a$  and  $d$  have the same parity.

## 6.6. Expected Losses

For convenience, recall the definition of the normal matrix as  $N = (I - Q)^{-1}$ . Using the matrix  $NR$  allows calculation of the expected values and variances for the losses that the attacker and defender will suffer in a war. For example, suppose  $A = 5$  and  $D = 4$ , as illustrated in Figure 6.1. In this case, the first row of the  $20 \times 9$  matrix  $NR$  gives the probabilities for the  $A + D = 9$  absorbing states:  $(NR)_{1,\cdot} = (0.138, 0.165, 0.179, 0.107, 0.050, 0.070, 0.124, 0.104, 0.064)$ . Let  $S_A$  and  $S_D$  denote the number of armies surviving for the attacker and defender respectively given the initial state  $X_0 = (A, D)$ . The probability distributions for  $S_A$  and  $S_D$



**Figure 6.5.** The probability mass function of absorbing states for  $A = 20$ ,  $D = 20$ . The absorbing states are in decreasing order of preference for the attacker.

are in the first row of  $NR$ :

$$\mathbb{P}[S_A = \ell] = \begin{cases} \sum_{\nu=A+1}^{A+D} (NR)_{1,\nu} & \text{if } \ell = 0, \\ (NR)_{1,A+1-\ell} & \text{if } \ell = 1, 2, \dots, A. \end{cases}$$

and

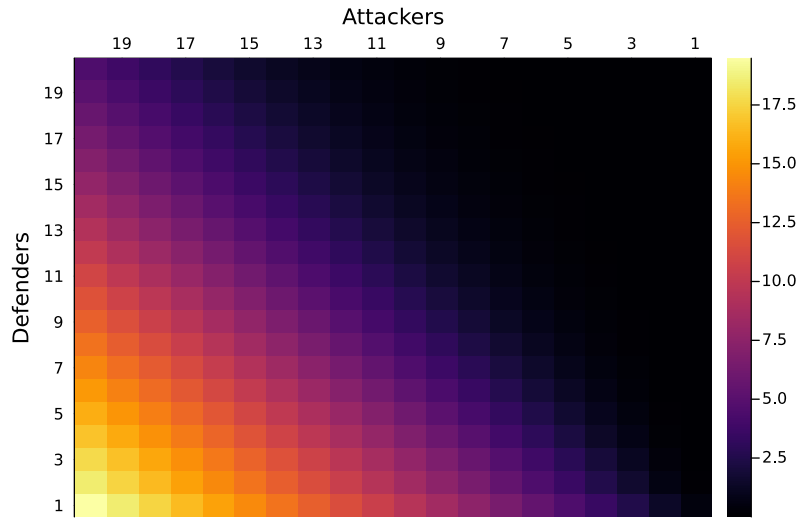
$$\mathbb{P}[S_D = \ell] = \begin{cases} \sum_{\nu=1}^A (NR)_{1,\nu} & \text{if } \ell = 0, \\ (NR)_{1,\ell} & \text{if } \ell = A+1, A+2, \dots, A+D. \end{cases}$$

For  $A = 5$  and  $D = 4$  the mean and standard deviation for the attacker's surviving armies are  $\mathbb{E}[S_A] = 2.15$  and  $\sqrt{\text{Var}[S_A]} = 1.89$ . The defender's mean and standard deviation in this case are  $\mathbb{E}[S_D] = 0.885$  and  $\sqrt{\text{Var}[S_D]} = 1.32$ . The attacker has an advantage in the sense that expected losses, 2.85, are lower than for the defender, 3.115. This is generally true provided the initial number of attacking armies is not too small.

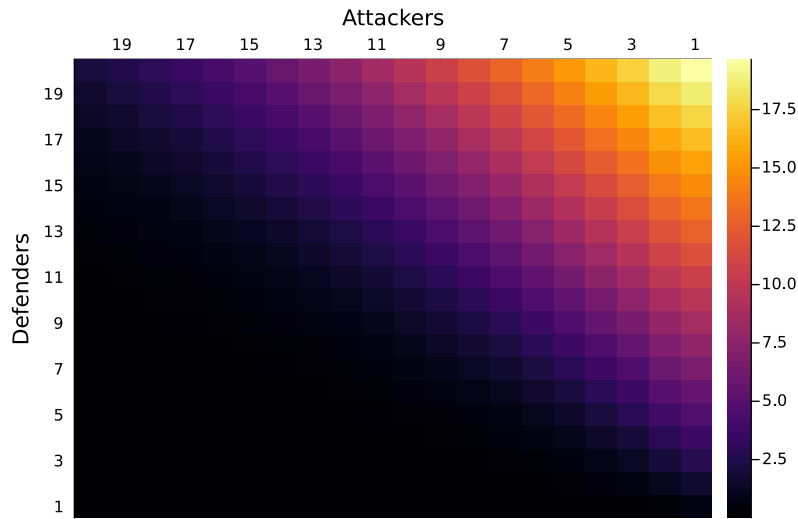
To get an overall sense of the number of armies remaining after a war, Figures 6.6 and 6.7 have heatmaps of expected surviving armies for values of  $A$  and  $D$  from 1 to 20. A heatmap is a graphical representation of data where the individual values contained in a matrix are represented as colors. Here the lighter colors represent larger numbers of armies surviving, the darker colors smaller number of armies. The matrix is the number of armies surviving after a war between a number of attackers along a column and defenders along a row. The scripts calculate the expected number of armies surviving.

When the number of attacking and defending armies is equal, the probability that the attacker ends up winning the territory exceeds 50%, provided the initial stakes are high enough, at least 5 armies each, initially, see Table 6.5. With 40 armies attacking 40 defending armies, the expected armies surviving are 7.5 attacking armies and 2.1 defending armies. The overall conclusion is that the chances of winning a war are more favorable for the attacker. The logical recommendation is for the attacker to be aggressive.

Using the absorption probabilities for the states  $(a, 0)$  where the attacker wins allows a more detailed summary of the outcomes of the war. As an example, suppose



**Figure 6.6.** Expected surviving attacking armies after starting with  $A$  attacking armies and  $D$  defending armies. Lighter colors represent larger numbers of armies surviving, the darker colors smaller numbers of armies. Note the axis scales, the number of attackers decrease left to right, the number of defenders decrease top to bottom, as in Figure 6.1



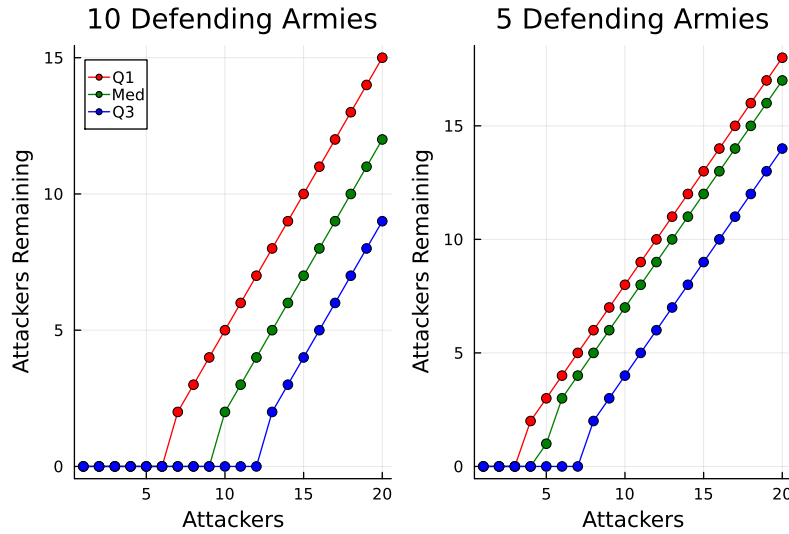
**Figure 6.7.** Expected surviving defending armies after starting with  $A$  attacking armies and  $D$  defending armies. Lighter colors represent larger numbers of armies surviving, the darker colors smaller numbers of armies. Note the axis scales, the number of attackers decrease left to right, the number of defenders decrease top to bottom, as in Figure 6.1.

20	19	18	17	16	15	14	13	12	11
0.633	0.628	0.623	0.617	0.611	0.605	0.599	0.592	0.584	0.576
10	9	8	7	6	5	4	3	2	1
0.568	0.558	0.547	0.536	0.521	0.506	0.477	0.470	0.363	0.417

**Table 6.5.** Probability of attacker winning when the number of armies are equal.

the attacker wants at least a probability of 0.75 of winning the war with at least four armies surviving. With how many armies should the attacker start a war to create this favorable situation? Refer to Figure 6.8 for an example of how to answer this important strategic question. Each facet in the figure indicates the number of defending armies, 10 or 5. The horizontal axis in each facet lists the number of starting attacking armies, while the vertical axis in each facet displays how many attacking armies survive after the war. Respectively, the blue, green and red curves with points indicate the first-quartile, median, and third-quartile states in the distribution of outcomes based on the number of the attacker's starting armies. The outcomes are in descending order of preference for the attacker. There are several ways to read the graphs. For example, consider the left facet corresponding to the defender starting with 10 armies. If the attacker starts with 15 armies, the most desired outcome is the absorbing state  $(15, 0)$ , while the least desired is  $(0, 10)$ . In this case, reading the chart vertically at  $a = 15$ , the median outcome is  $(7, 0)$  in the sense that  $(a, 0)$  with  $a \geq 7$  has a probability of at least 0.50 (in fact,  $\mathbb{P}[a \geq 7, d = 0] = 0.571$ .) This means that with probability at least 0.50, the attacker will finish the war with 7 or more armies. The interquartile range is  $(4, 0)$  through  $(10, 0)$ . This means that with probability at least 0.25 (the probability is 0.290) the attacker will win the war and have 10 or more armies surviving; with probability at least 0.50 (the probability is 0.579) the attacker will win and have 4 to 10 armies surviving; and the surviving 0.25 probability (the probability is 0.218) of battles will leave the attacker with 4 or fewer armies. Returning to the question of how many armies the player needs to start with to attack a defender with 5 armies with at least a probability of 0.75 of winning with at least 4 armies remaining, reading the second chart horizontally, the attacker should start with at least 10 armies. The figure and the prior examples are illustrative, using up to 20 attacking armies with 10 or 5 defending armies. The script below shows how to calculate these quartiles for any number of attackers and defenders.

The number of battles fought in a war is the number of dice rolls until absorption into one of the states  $(a, 0)$  or  $(0, d)$ . This is the number of state transitions to absorption, also called the waiting time until absorption. The standard formula for calculating the expected waiting time to absorption is  $(I - Q)^{-1}\mathbf{1}$ . Using this, the expected number of battles for a war with 10 attacking armies against 4 defending armies is 3.994. The R script below shows how to calculate the expected waiting time to absorption for any number of attackers and defenders.



**Figure 6.8.** Quartile statistics for the number of attacking armies surviving from 10 defending armies and 5 defending armies.

## 6.7. Chapter Ending Answer

The order statistics are  $Y^{(3)}$ , the largest value among  $Y_1, Y_2, Y_3$ ;  $Y^{(2)}$ , the second largest value, including ties, among  $Y_1, Y_2, Y_3$ ; and  $Y^{(1)}$ , the largest value, including ties, among  $Y_1, Y_2, Y_3$ .

## 6.8. Chapter Summary

### Key Concepts.

- (1) *Risk* is a board game of wars between two players, and each war consists of one or more rounds of combat between  $A$  attacking armies and  $D$  defending armies. The goal is to develop the probability of winning the war as a function of  $A$  and  $D$  using a Markov chain with  $AD + A + D$  states.

### Vocabulary.

- (1) Given a sample of  $n$  identically distributed random values, the  $\ell$ th **order statistic** is the  $\ell$ th largest value.

### Notation.

- (1)  $A$  – the number of attacking armies
- (2)  $D$  – the number of defending armies
- (3)  $X_n$  – the state of the system at the beginning of the  $n$ th turn:

$$X_n = (a_n, d_n), 0 \leq a_n \leq A, 0 \leq d_n \leq D$$

where  $a_n$  and  $d_n$  are the number of attacking and defending armies respectively

- (4)  $\rho_{ij\ell}$  – the joint probabilities associated with the best and second best roll from 2 or 3 six-sided fair dice
- (5)  $Y_1, Y_2, Y_3$  – the unordered outcome for an attacker when rolling three dice
- (6)  $W_1, W_2$  – the unordered outcome for an attacker when rolling two dice
- (7)  $Z_1, Z_2$  – the unordered outcome for a defender rolling two dice
- (8)  $Y^{(1)} \geq Y^{(2)} \geq Y^{(3)}$  – the ordered random variables are the *order statistics*
- (9)  $f_{ij}^{(n)}$  – the probability that the first (and final) visit from state  $i$  to absorbing state  $j$  occurs on the  $n$ th turn
- (10)  $F^{(n)}$  –  $AD \times (A + D)$  matrix of these first transitions
- (11)  $F = (I - Q)^{-1}R$  – probability that the system eventually goes from transient state  $i$  to absorbing state  $j$
- (12)  $R_A$  and  $R_D$  – the number of armies remaining for the attacker and defender respectively given the initial state  $X_0 = (A, D)$  probabilities

## 6.9. Sources

This chapter on *Risk* is adapted from [Os03], [PW15] and [Tan97].

## 6.10. Algorithms and Scripts

q

**Data:** Maximum number of attacking and defending armies

**Result:** Absorption probabilities and win probabilities

- 1 **function** stateToIndex ( $a, d$ )
- 2 Given a state, return the index for the transition probability matrix
- return** index
- 3 **function** indexToState ( $n$ )
- 4 Given an index for the Markov chain, return the state ( $a, d$ )
- 5 **return** State
- 6 *Initialization of Matrices*
- 7 Define 14 transition probabilities
- 8 Fill transition probability matrix
- 9 *Markov chain calculations*
- 10 Load Markov Chain library
- 11 Create *Risk* Markov chain object
- 12 Find absorption probabilities of *Risk* game chain
- 13 Sum up attacker and defender win probabilities

**Algorithm 8:** Risk Markov chain

**R:**

```

1
2 A <- 10
3 D <- 4
4 ## A <- 40
```

```

5 ## D <- 40
6
7 totalStates <- A * D + (A + D)
8
9 stateToIndex <- function(a,d) {
10   # given a state, return the index for the trans
   prob matrix
11   if (a > 0) {
12     ind <- (A+1 - a) + (D-d)*A
13   } else {
14     ind <- A*D + A + d
15   }
16   ind
17 }
18
19 indexToState <- function(ind) {
20   # given an index for a transient state, return
   the state as a pair
21   if (ind <= A*D + A) {
22     j <- A*D - ind
23     r <- j %% A
24     first <- 1 + r
25     second <- 1 + (j-r)/A
26   } else {
27     first <- 0
28     second <- ind - (A*D + A)
29   }
30   c(first, second)
31 }
32
33 rho111 <- 15/36 # light gray
34 rho110 <- 21/36 # magenta
35
36 rho121 <- 55/216 # brown
37 rho120 <- 161/216 # purple
38
39 rho211 <- 125/216 # pink
40 rho210 <- 91/216 # black
41
42 rho222 <- 295/1296 # cyan
43 rho221 <- 420/1296 # darkgreen
44 rho220 <- 581/1296 # yellow
45
46 rho311 <- 855/1296 # orange
47 rho310 <- 441/1296 # gray
48
49 rho322 <- 2890/7776 # green

```



```

50 rho321 <- 2611/7776                                # blue
51 rho320 <- 2275/7776                                # red
52
53 QR <- matrix(0, A * D, A * D + A + D)
54 ## R <- matrix(0, A * D, A + D)
55 I <- diag(A + D)
56 Z <- matrix(0, A + D, A * D)
57
58 att3dice <- seq(from=A, to = 3, by=-1)
59 def2dice <- seq(from=D, to = 2, by=-1)
60
61 # Cases 6, 5, 4
62 for (d in def2dice) {
63   for (a in att3dice) {
64     QR[stateToIndex(a,d), stateToIndex(a, d-2)]
65     <- rho322 # green
66     QR[stateToIndex(a,d), stateToIndex(a-1, d-1)]
67     <- rho321 # blue
68     QR[stateToIndex(a,d), stateToIndex(a-2, d)]
69     <- rho320 # red
70   }
71   QR[stateToIndex(2, d), stateToIndex(2, d-2)] <-
72   rho222 # cyan
73   QR[stateToIndex(2, d), stateToIndex(1, d-1)] <-
74   rho221 # darkgreen
75   QR[stateToIndex(2, d), stateToIndex(0, d)] <-
76   rho220 # yellow
77
78   QR[stateToIndex(1, d), stateToIndex(1, d-1)] <-
79   rho121 # purple
80   QR[stateToIndex(1, d), stateToIndex(0, d)] <-
81   rho120 # brown
82 }
83
84 # Case 3
85 for (a in att3dice) {
86   QR[stateToIndex(a, 1), stateToIndex(a, 0)] <-
87   rho311 # orange
88   QR[stateToIndex(a, 1), stateToIndex(a-1, 1)] <-
89   rho310 # gray
90 }
91
92 # Cases 2 and 1
93 QR[stateToIndex(2, 1), stateToIndex(2, 0)] <- rho211
94   # pink
95 QR[stateToIndex(2, 1), stateToIndex(1, 1)] <- rho210
96   # black

```

```

85 QR[stateToIndex(1, 1), stateToIndex(1, 0)] <- rho111
   # lightgray
86 QR[stateToIndex(1, 1), stateToIndex(0, 1)] <- rho110
   # magenta
87
88 M <- rbind(QR, cbind(Z, I))
89
90 library("markovchain")
91
92 riskChain <- new("markovchain", states = as.character
   (1:totalStates), byrow = TRUE,
93   transitionMatrix = M, name = "RISK")
94 absorpProb <- absorptionProbabilities(riskChain)
95 attackerWins <- apply(absorpProb[, 1:A], 1, sum)
96 attackerWinTable <- t(matrix(formatC(attackerWins,
   digits=3, format="f"), A,D))

```

```

R:
1 A <- 20
2 D <- 20
3
4 totalStates <- A * D + (A + D)
5
6 stateToIndex <- function(a,d) {
7   # given a state, return the index for the trans
   prob matrix
8   if (a > 0) {
9     ind <- (A+1 - a) + (D-d)*A
10  } else {
11    ind <- A*D + A + d
12  }
13  ind
14 }
15
16 indexToAttackers <- function(ind) {
17   # for transient state index, return number of
   Attacking armies
18   j <- A*D - ind
19   r <- j %% A
20   attArmies <- 1 + r
21   attArmies
22 }
23
24 indexToDefenders <- function(ind) {
25   # given an index for a transient state, return
   number of Defending armies
26   j <- A*D - ind

```

```

27     r <- j %% A
28     defArmies <- 1 + (j-r)/A
29     defArmies
30 }
31
32 indexToState <- function(ind) {
33     # given an index for a transient state, return
34     # the state as a pair
35     if (ind <= A*D + A) {
36         j <- A*D - ind
37         r <- j %% A
38         first <- 1 + r
39         second <- 1 + (j-r)/A
40     } else {
41         first <- 0
42         second <- ind - (A*D + A)
43     }
44     c(first, second)
45 }
46
47 rho111 <- 15/36 # light gray
48 rho110 <- 21/36 # magenta
49
50 rho121 <- 55/216 # brown
51 rho120 <- 161/216 # purple
52
53 rho211 <- 125/216 # pink
54 rho210 <- 91/216 # black
55
56 rho222 <- 295/1296 # cyan
57 rho221 <- 420/1296 # darkgreen
58 rho220 <- 581/1296 # yellow
59
60 rho311 <- 855/1296 # orange
61 rho310 <- 441/1296 # gray
62
63 rho322 <- 2890/7776 # green
64 rho321 <- 2611/7776 # blue
65 rho320 <- 2275/7776 # red
66
67 QR <- matrix(0, A * D, A * D + A + D)
68 ## R <- matrix(0, A * D, A + D)
69 I <- diag(A + D)
70 Z <- matrix(0, A + D, A * D)
71
72 att3dice <- seq(from=A, to = 3, by=-1)
73 def2dice <- seq(from=D, to = 2, by=-1)

```

```

73
74 # Cases 6, 5, 4
75 for (d in def2dice) {
76   for (a in att3dice) {
77     QR[stateToIndex(a,d), stateToIndex(a, d-2)]
78     <- rho322 # green
79     QR[stateToIndex(a,d), stateToIndex(a-1, d-1)]
80     <- rho321 # blue
81     QR[stateToIndex(a,d), stateToIndex(a-2, d)]
82     <- rho320 # red
83   }
84   QR[stateToIndex(2, d), stateToIndex(2, d-2)] <-
85   rho222 # cyan
86   QR[stateToIndex(2, d), stateToIndex(1, d-1)] <-
87   rho221 # darkgreen
88   QR[stateToIndex(2, d), stateToIndex(0, d)] <-
89   rho220 # yellow
90
91   QR[stateToIndex(1, d), stateToIndex(1, d-1)] <-
92   rho121 # purple
93   QR[stateToIndex(1, d), stateToIndex(0, d)] <-
94   rho120 # brown
95 }
96
97 # Cases 3
98 for (a in att3dice) {
99   QR[stateToIndex(a, 1), stateToIndex(a, 0)] <-
100   rho311 # orange
101   QR[stateToIndex(a, 1), stateToIndex(a-1, 1)] <-
102   rho310 # gray
103 }
104
105 # Cases 2 and 1
106 QR[stateToIndex(2, 1), stateToIndex(2, 0)] <- rho211
107 # pink
108 QR[stateToIndex(2, 1), stateToIndex(1, 1)] <- rho210
109 # black
110 QR[stateToIndex(1, 1), stateToIndex(1, 0)] <- rho111
111 # lightgray
112 QR[stateToIndex(1, 1), stateToIndex(0, 1)] <- rho110
113 # magenta
114
115 M <- rbind(QR, cbind(Z, I))
116
117 library("markovchain")

```

```

105 riskChain <- new("markovchain", states = as.character
    (1:totalStates), byrow = TRUE,
106     transitionMatrix = M, name = "RISK")
107 absorpProb <- absorptionProbabilities(riskChain)
108
109 ## Now I calculate the expected number of Attacking
    armies remaining
110 ## from each state. This is the inner or dot product
    of the submatrix
111 ## absorpProb[ , 1:20] with the vector 20:1. Note
    that the first column
112 ## of absorpProb[ , 1:20] is 20 Attacker armies
    remain, the second column of
113 ## absorpProb[ , 1:20] is 19 Attacking armies remain
    and so on.
114 ## This explains the use of the descending vector
    20:1.
115 ## Furthermore, for example consider row 90, which
    corresponds to
116 ## state Att = 11 and Def = 16. Then examination of
    the product shows
117 ## the first 9 entries of absorpProb[90, 1:20] are 0,
    positive probabilities
118 ## only start at entry 16, as described in the text,
    so the only contribution
119 ## to the expected number of attacking armies
    remaining will be from the
120 ## absorption probabilities of 11, 10, 9, ..., 1
    armies remaining.
121
122 attArmiesRemain <- absorpProb[ , 1:20] %*% 20:1
123
124 attackersRemain = data.frame(Att=indexToAttackers
    (1:400),
125                               Def=indexToDefenders
    (1:400),
126                               attRem=attArmiesRemain)
127
128 defArmiesRemain <- absorpProb[ , 21:40] %*% 1:20
129
130 defendersRemain = data.frame(Att=indexToAttackers
    (1:400),
131                               Def=indexToDefenders
    (1:400),
132                               defRem=defArmiesRemain)
133
134 ## library("ggplot2")

```

```

135 ## ggplot(attackersRemain, aes(Att,Def)) +
136 ##     geom_raster(aes(fill=attRem)) +
137 ##     scale_x_reverse() +
138 ##     xlab("Attackers") +
139 ##     ylab("Defenders") +
140 ##     scale_fill_viridis_c()
141
142 ## ggplot(defendersRemain, aes(Att,Def)) +
143 ##     geom_raster(aes(fill=defRem)) +
144 ##     scale_x_reverse() +
145 ##     xlab("Attackers") +
146 ##     ylab("Defenders") +
147 ##     scale_fill_viridis_c()

```

. language=R

## 6.11. Problems to Work for Understanding

Chapter 6: The Game of Risk as a Markov Chain.

6.1: Given the values  $Y_1, Y_2, Y_3$  from a roll of 3 dice, show that the probability for  $Y^{(1)} = y^{(1)}, Y^{(2)} = y^{(2)}$  with  $y^{(1)} > y^{(2)}$  is  $\frac{6y^{(2)}-3}{216}$ .

6.2: Given the values  $Y_1, Y_2, Y_3$  from a roll of 3 dice, show that the probability for  $Y^{(1)} = y^{(1)}$  show the marginal distribution of the best roll is

$$\mathbb{P}\left[Y^{(1)} = y^{(1)}\right] = \frac{1 - 3y^{(1)} + 3(y^{(1)})^2}{216}$$

for  $y^{(1)} = 1, 2, 3, 4, 5, 6$ .

6.3: For the game of *Risk*, show that the probability of the attacker rolling three dice, the defender rolling one die and the defender losing one army is  $855/1296$ . That is, calculate  $\rho_{311}$ , the orange arrow in Figure 6.1 and Table 6.3.

6.4: Find the expected number of attacking armies remaining when attacking an equal number of defending armies, for  $n = 20$  to  $n = 1$ .



## Games as Markov Chains

This chapter examines 4 additional games as Markov chains. The goal is to determine the expected number of moves or plays to reach a winning state. The games have from 11 states to 165 states and another goal is to show how to construct the states and the transition probability matrices in these cases.

Mathematically Mature: contains mathematics beyond calculus with proofs.

### 7.1. Chapter Starter Question

What feature of a board game is necessary for it to be modeled as a Markov chain? Can you think of a board game that can be modeled as a Markov chain? What would be an example of a game which cannot be modeled as a Markov chain?

### 7.2. Tenzi

*Tenzi* is a simple dice game for multiple players. Each player starts with 10 six-sided fair dice. For a round, one player calls out, e.g., “Tenzi Four!” Each player rolls all the dice in their hands as quickly as possible. Whenever a “four” comes up, the player sets it aside and rolls all the remaining dice again. Eventually the player achieves all 10 “fours” and calls out “Tenzi!”, becoming the winner of the round.

A Markov chain models the game-play of *Tenzi* for a single player. Each state in the Markov chain represents the player’s accumulated number of dice matching the target number. So at any point in the game, a player will be in one of the 11 states  $\{0, 1, 2, 3, \dots, 10\}$ . A player in state 0 has not yet rolled any dice matching the target number, and a player in state 10 will call out “Tenzi!” Each time a player rolls the dice, the player has a chance to remain in the current state or to move up to a higher-numbered state.

Each entry in the transition probability matrix is a binomial probability. A player in state  $i$  rolls the remaining  $10 - i$  dice. The player moves to state  $j \geq i$  if



exactly  $j - i$  of the dice match the target number. The probability of transitioning from state  $i$  to state  $j$  in one roll of the dice is  $\binom{10-i}{j-i} \left(\frac{1}{6}\right)^{j-i} \left(\frac{5}{6}\right)^{10-j}$  for  $0 \leq i \leq j \leq 10$ . A player will never go backwards to a previous state in the game, so the probability is 0 for  $i > j$ . Thus the states are not communicating, the Markov Chain is not recurrent, states 0 through 9 are transient and the state 10 is an absorbing state.

The full  $11 \times 11$  transition probability matrix  $P$  is approximately

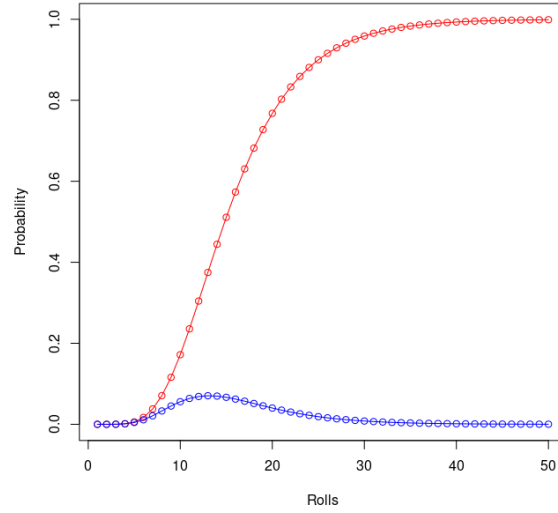
$$P = \begin{pmatrix} 0.16 & 0.32 & 0.29 & 0.16 & 0.054 & 0.013 & 0.0022 & 2.5E-4 & 1.9E-5 & 8.3E-7 & 1.7E-8 \\ 0.0 & 0.19 & 0.35 & 0.28 & 0.13 & 0.039 & 0.0078 & 0.0010 & 8.9E-5 & 4.5E-6 & 9.9E-8 \\ 0.0 & 0.0 & 0.23 & 0.37 & 0.26 & 0.10 & 0.026 & 0.0042 & 4.2E-4 & 2.4E-5 & 6.0E-7 \\ 0.0 & 0.0 & 0.0 & 0.28 & 0.39 & 0.23 & 0.078 & 0.016 & 0.0019 & 1.3E-4 & 3.6E-6 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.34 & 0.40 & 0.20 & 0.054 & 0.0080 & 6.4E-4 & 2.1E-5 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.40 & 0.40 & 0.16 & 0.032 & 0.0032 & 1.3E-4 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.48 & 0.39 & 0.12 & 0.015 & 7.7E-4 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.58 & 0.35 & 0.069 & 0.0046 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.69 & 0.28 & 0.028 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.83 & 0.17 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{pmatrix}$$

rounding to 2 significant figures and using calculator-style notation  $2.5E-4 = 2.5 \times 10^{-4}$  to conserve space. The initial distribution is  $X_0 = (1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$ . The value in the last place of  $X_n = X_0 P^n$  is the probability of reaching the absorbing or winning state for Tenzi in  $n$  or fewer rolls. For example, the value in the last entry of  $X_{20}$  is 0.768. The player has a 76.8% chance the game finishes by the 20th roll. The player may have finished on the 20th roll, or possibly finished on some previous roll and is waiting in absorbing state 10. The resulting cumulative probability function  $P(j)$  for a player getting Tenzi on or before the  $j$ th roll is in Figure 7.1. To find  $p(j)$ , the probability of getting Tenzi in exactly  $j$  rolls, subtract the probability that the player already had Tenzi by the  $j - 1$  roll. This gives the probability density function  $p(j) = P(j) - P(j - 1)$  also shown in Figure 7.1. The maximum of this probability function is at  $j = 13$ ; a player has a 0.0705 probability of getting Tenzi on the 13th roll. Using these probabilities, the mean of the distribution is  $\sum_{j=1}^{\infty} jp(j)$ . Approximate this sum through  $j = 50$  as 16.5. This is the average number of rolls needed for a player to get Tenzi.

The fundamental matrix  $N = (I - Q)^{-1}$  provides another way of finding the mean. The transition probability matrix is already partitioned as

$$P = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix}$$

where  $Q$  is the  $10 \times 10$  matrix containing the transition probabilities among the transient states,  $R$  is a  $10 \times 1$  column matrix containing the probabilities of going from each of the non-absorbing states to state 10 in one roll,  $0$  is a  $1 \times 10$  zero matrix, and  $I$  is the  $1 \times 1$  identity matrix representing the absorbing state 10.



**Figure 7.1.** Probability density function (in blue) and cumulative distribution function (in red) of waiting time to win in Tenzi.

Then  $N$  is approximately

$$\begin{pmatrix} 1.193 & 0.478 & 0.669 & 0.787 & 0.915 & 1.097 & 1.371 & 1.828 & 2.742 & 5.485 \\ 0.000 & 1.240 & 0.564 & 0.771 & 0.917 & 1.097 & 1.371 & 1.828 & 2.742 & 5.485 \\ 0.000 & 0.000 & 1.303 & 0.673 & 0.905 & 1.099 & 1.371 & 1.828 & 2.742 & 5.485 \\ 0.000 & 0.000 & 0.000 & 1.387 & 0.815 & 1.091 & 1.373 & 1.828 & 2.742 & 5.485 \\ 0.000 & 0.000 & 0.000 & 0.000 & 1.504 & 1.010 & 1.368 & 1.829 & 2.742 & 5.485 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 1.672 & 1.298 & 1.826 & 2.743 & 5.485 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 1.931 & 1.769 & 2.742 & 5.485 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 2.374 & 2.697 & 5.485 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 3.273 & 5.455 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 6.000 \end{pmatrix}.$$

The theorems from the chapter on Waiting Time to Absorption give a lot of information about the progress of the game. The entry  $N_{ij}$  (counting  $i$  and  $j$  from 0) represents the expected number of turns spent in state  $j$  given that the player started in state  $i$ . Notice that the diagonal entries are all greater than 1. If a player starts the game in state  $i$  then at least one roll, the first roll, is in state  $i$ . Entries in later states  $j > i$  can be less than 1 because it is possible for a player to skip a state entirely. Notice the 6 in the bottom right corner gives the average number of rolls spent in state 9 given that the player started in state 9. This makes sense; in state 9, the player has just one die left to roll. It will take 6 rolls on average to roll the given target number, this is the mean of a geometric random variable with  $p = 1/6$ . Since players start the game of *Tenzi* in state 0 the first row of matrix  $N$  gives the expected number of rolls a player will spend in each state, see Table 7.1. This makes sense, for state 0, there is always the first roll, but usually the player

State	0	1	2	3	4	5	6	7	8	9
Rolls	1.19	0.48	0.67	0.79	0.92	1.10	1.37	1.83	2.74	5.48

**Table 7.1.** Expected number of times the chain will be in each state.

State	0	1	2	3	4	5	6	7	8	9
SD	6.83	6.81	6.78	6.75	6.70	6.64	6.55	6.41	6.14	5.48

**Table 7.2.** Standard deviation of the number of times the chain will be in each state.

moves to another state. For states 1 through 4, it is common to get more than one of the target number, so those states often get skipped over. For states 5 to 9, it takes increasingly longer to collect the target number.

The sum of the first row is the mean number of turns to go from state 0 to the absorbing state 10, specifically, 16.564849, agreeing with the approximate mean from the p.d.f. The standard deviation of the number of turns the player will spend in state  $i$  before reaching the absorbing state 10 from state 0 is in Table 7.2. The scripts provide the calculations for these standard deviations. This also makes sense; in state 9, then a player has just one die left to roll. The entry 5.48 is the approximate standard deviation of a geometric random variable with  $p = 1/6$ .

### 7.3. Random Moves in the Towers of Hanoi

The Towers of Hanoi (also called the Tower of Brahma or Lucas' Tower) is a mathematical game or puzzle. It consists of three rods and some number of disks of different sizes, with holes in the center so each disk can slide onto any rod. The puzzle starts with the disks in a neat stack in ascending order of size on one rod, the smallest at the top, making a conical shape. The objective of the puzzle is to move the entire stack to another rod, obeying 3 rules.

- (1) Only one disk can be moved at a time.
- (2) Each move consists of taking the top disk from one of the stacks and placing it on top of another stack or on an empty rod.
- (3) No larger disk may be placed on top of a smaller disk.

Consider solving the small three disk case of Lucas' Tower puzzle with random legal moves. The disks start with the biggest disk at the bottom, the intermediate size disk in the middle, and the smallest disk on top. The goal is to move all three disks, one at a time, from one pole to another pole. At no point can a larger disk sit atop a smaller disk. See Figure 7.2

The minimum number of moves to solve the puzzle is well known:  $m$  disks can be solved in exactly  $2^m - 1$  moves. The maximum number of legal moves to move all three disks from one pole to any other pole without repeating a configuration is  $3^m - 1$ . The question here is: on average, how many moves does it take to solve this puzzle with *random* legal moves of three disks?



**Figure 7.2.** Starting configuration and a typical state in the Towers of Hanoi puzzle.

Label the rods from left to right as  $a, b, c$  as in Figure 7.2. Represent the states for 3 disks as a triplet of values from  $\{a, b, c\}$ . The first entry in the triplet gets the rod label on which the smallest disk rests, the second entry in the triplet gets the rod label for the middle disk, and the third entry in the triplet gets the rod label on which the largest disk rests. So the start is  $aaa$ , the goal is either  $bbb$  or  $ccc$ . The configuration  $aba$  implies the smallest disk is on top of the largest disk, while the medium disk is on the middle rod labeled  $b$ . The puzzle with 3 disks has 27 legal configurations.

The triplet labeling leads to an example of a *puzzle graph*, in which the configurations of a puzzle or game are the nodes of a graph and legal moves between states are the edges of the puzzle graph. Figure 7.3 is the puzzle graph for the Towers of Hanoi. For example, the edge connecting  $aaa$  with  $baa$  represents the initial move of the smallest disk to the middle rod. The puzzle graph for the Towers of Hanoi has a recursive ternary structure useful for analyzing the shortest and longest paths from the start  $aaa$  to the goals  $bbb$  or  $ccc$ . For this small random game just number the states from the source, top to bottom, left to right, as in Figure 7.3

Selecting each move uniformly randomly from the set of all valid moves from any node to any adjacent node (except for the goal nodes which are absorbing) defines a random walk on the graph or a Markov chain. The two goals, now states 20 and 27, are absorbing states. Most transition probabilities between states are  $1/3$ , except for the start and end states. The recursive ternary labeling of the nodes is not immediately useful for analysis of this 27-state Markov chain. A script for this Markov chain calculates the mean absorption time as 70.77 moves, see the exercises. T. Berger and M. Alekseyev [AB15] give two proofs that the mean time to absorption for the  $m$ -disk Tower of Hanoi puzzle with random moves is

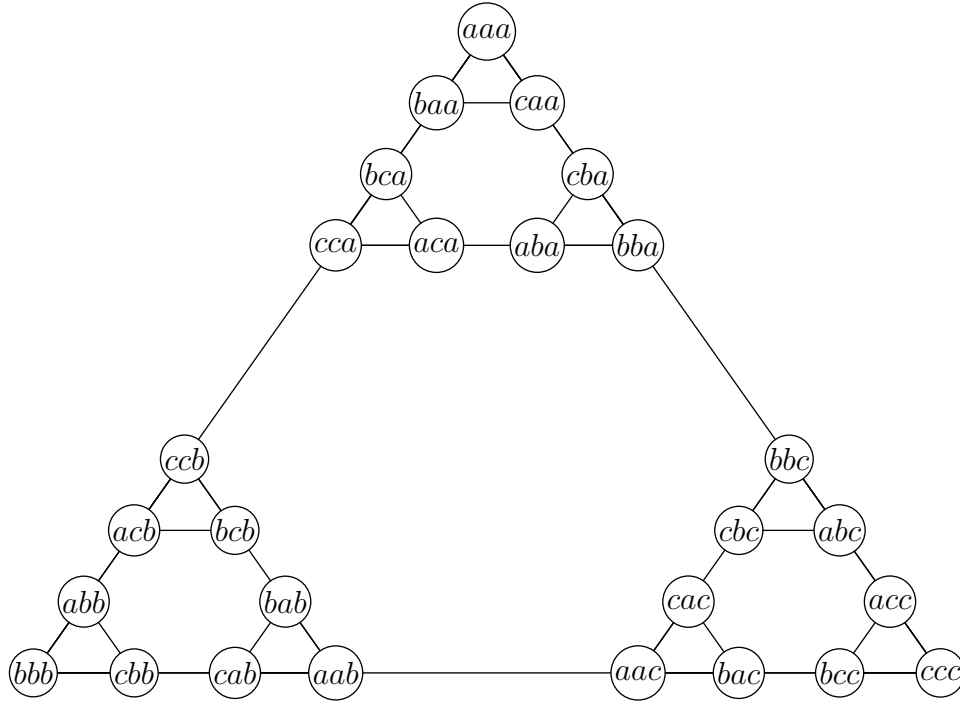
$$\frac{(3^m - 1)(5^m - 3^m)}{4 \cdot 3^{m-1}}.$$

One proof uses recurrence relations, the other proof uses an equivalence of Markov chains to electrical networks.

## 7.4. Chutes and Ladders

The children's' game *Chutes and Ladders* (known in the United Kingdom as *Snakes and Ladders*) derives from an old Hindu game *Leela* or *Moksha Patam* teaching moral lessons. The game described here is the modified U.S. version. The game is a 100 state absorbing Markov chain and the goal is to investigate the expected playing time.

The game is for two or more players. The game play is on a 10 by 10 board with squares numbered 1 to 100 that are the states of the game. Rather than



**Figure 7.3.** The puzzle graph for the three disk Towers of Hanoi.

add an additional state 0 as the starting position, instead make an initial uniform distribution on the 6 possible starting states, see below for details. (The scripts, in languages which index vectors from 1 in contrast to Python which indexes from 0, motivate this choice of 100 states with an initial distribution. With 101 states including a starting state, the state indices in scripts would be one greater than the spaces marked on the board, leading to potential confusion.) Since the goal is to find the expected playing time, add 1 to the playing time for the initial move to be in one of the starting states. Players roll a fair six-sided die (or use a fair six-section spinner) to determine how many squares to advance their token on each turn. Two or more players may occupy the same square simultaneously. The first player to reach square 100 exactly wins. In the final 5 states, if a move would take a player beyond the last square, the player does not move. The game board is also marked with chutes and ladders connecting various squares on the board. The special feature of the game is that if a token lands on a square at the bottom of a ladder the token immediately moves to the top of the ladder. Similarly if the token lands on a square at the top of a chute, it immediately moves to the bottom of the chute. The game has 10 chutes and 9 ladders with beginning and end states given by the following ordered pairs

- Ladders: (1, 38), (4, 14), (9, 31), (21, 42), (28, 84), (36, 44), (51, 67), (71, 91), (80, 100);

- Chutes: (16, 6), (47, 26), (49, 11), (56, 53), (62, 19), (64, 60), (87, 24), (93, 73), (95, 75), (98, 78).

This means that 19 states, the beginnings of the chutes and ladders, are inaccessible states. A player is never actually in state 1, for if the token lands on square 1, the ladder (1, 38) immediately deposits the player into state 38. Although the game is a race among two or more players, the players move independently, so it is sufficient to consider just one player moving and ask “How long does it typically take a single player to finish a game by reaching square 100?”

Although the game has 100 squares, it is possible to model the game as a Markov chain with fewer states, see [AKS93]. Adding a starting state 0, but deleting each inaccessible state corresponding to a chute or a ladder leaves 82 states. The transition probability matrix is an  $82 \times 82$  matrix with most rows containing 6 consecutive probabilities of  $1/6$  each. There are two kinds of exceptions. A row corresponding to any state reachable from a chute or ladder must account for the long-distance transitions by the chute or ladder. The last 5 rows show the fact that a player must reach state 100 exactly, a die roll causing the player to go past state 100 results in no move.

Here the model uses a 100-state Markov chain with a  $100 \times 100$  transition probability matrix derived from matrices analogous to those in the Monopoly model. First use a  $100 \times 100$  circulant (almost, excepting the last 5 rows) dice roll matrix  $R$  followed by sparse  $100 \times 100$  chutes and ladders transition matrices  $C$  and  $L$ . The matrix  $L$  is just the identity matrix but, for instance the 1 in row 1 and column 1, moves to row 1 and column 38 to indicate ladder (1, 38). Likewise for the 18 other ladders and chutes. The result  $RLC$  is a  $100 \times 100$  transition probability matrix with transient states 1 through 99 and absorbing state 100. The game starts in states 38, 2, 3, 14, 5 and 6, each with probability  $\frac{1}{6}$ . The expected waiting time to absorption is the average over the expected waiting time to absorption from each state,  $\frac{1}{6}(W(38) + W(2) + W(3) + W(14) + W(5) + W(6)) = 38.22512$ . Adding 1 for the initial move to the starting states gives 39.22512, agreeing with [AKS93]. Using Theorem 3.3 from Waiting Time to Absorption the standard deviation of the waiting time to absorption is approximately 25.2 turns. As a final note, observe that the waiting time to absorption from state 99 is 6 with standard deviation  $\sqrt{30} \approx 5.48$ , exactly as expected for a geometric random variable with  $p = 1/6$ , waiting to roll a 1 to enter the last state.

In [AKS93] the authors investigate the sensitivity of the waiting time to adding or removing chutes and ladders. For example, the expected waiting time to absorption for a game with no chutes and ladders is 31.1 moves. See the exercises for more examples.

## 7.5. Count Your Chickens

*Count Your Chickens!*, produced by Peaceable Kingdom, is a simple game for preschoolers. In this cooperative game, play begins with forty chicks spread throughout the board and a mama chicken at the start square. The end square is the mama chicken’s coop, and the mama chicken moves progressively closer to this square as the game unfolds. The object of the game is to have all 40 chicks in the chicken

coop when the mama chicken arrives there. The game board has 41 squares numbered in order, with 30 squares containing one of five characters: a cow, a sheep, a pig, a dog, or a tractor. The remaining 11 squares are empty and neutral. Five of the character squares have a blue background. The final square, the chicken coop, contains all 5 farm characters. Players take turns spinning a spinner with 6 segments of equal area. Five segments match the farm characters from the board and a sixth segment has a fox character. When a player spins the spinner, one of two things can happen. If the player spins one of the five characters drawn on the board, she moves the mama chicken token along the path toward the coop to the next instance of the character. The player counts the squares moved, and adds this number of chicks to the chicken coop. Additionally, if the square landed on has a blue background, the player adds one additional chick to the coop. There are only a total of 40 chicks on the board though, so if the mama chicken moves two squares but there are already 39 chicks in the coop, only one chick gets added. If a fox is spun, the player must remove one chick from the coop and place it back on the board. If there are no chicks in the coop then spinning a fox has no effect.

Suppose the mama chicken is at the start square. If the player spins a sheep, then the mama chicken moves to square 2 (the first sheep) and places two chicks in the coop. If the player next spins a tractor then the mama chicken moves 2 squares to square 4 and places 3 more chicks in the coop because square 4 is blue. If the first spin is a fox then nothing happens because at the start of the game there are no chicks in the coop. The game continues in this manner until the mama chicken reaches the coop. The players win if all 40 chicks are in the coop when the mama chicken arrives there; otherwise the players lose, this is a cooperative game.

The goal here is to answer the following questions:

- (1) What is the probability of winning a game of *Count Your Chickens!*? That is, what is the probability of landing on square 40 with 40 chicks in the coop?
- (2) What is the expected number of chicks in the coop at the end of the game?
- (3) What effect do the blue squares have on the probability of winning the game? For example, the original game has five particular squares colored blue; are there other choices of five blue squares that increase the probability of winning the game?

The mathematical interest here is creating the state space, leading to a large transition probability matrix. A state in *Count Your Chickens!* is an ordered pair  $(a, b)$  where  $a$  is the mama chicken's position on the board and  $b$  is the number of chicks in the coop. For win probabilities only, to minimize the number of states and cut down on computation, include a "loss" state and a "win" state. The idea is that while  $(39, 35)$ , for example, is a possible state of the game, it is impossible to win from such a configuration. Lump together all such ordered pairs from which it is impossible to win as a loss state. The win state is  $(40, 40)$ , the mama chicken must reach the last square of the board with all of the chicks in the coop.

The following illustrates construction of a chain from a smaller board, see Figure 7.4.

This smaller game uses only two farm characters – a sheep and a cow. There are 8 squares on the board after the start square and 8 chicks to return to the coop.

0 Start	1	2 Sheep	3 Cow	4	5 Cow	6	7 Sheep	8 Coop Sheep Cow
------------	---	------------	----------	---	----------	---	------------	------------------------

**Figure 7.4.** Smaller game board for the example *Count Your Chickens!*

The spinner has three equal-sized segments illustrated with a cow, a sheep, and a fox.

A state of the game is an ordered pair  $(i, j)$  where  $i$  is the position of the mama chicken and  $j$  is the number of chicks in the coop. Identify some pairs with the loss state because if  $j$  is small enough relative to the mama chicken's position, it will be impossible for all 8 chicks to be in the coop at the end of the game. The state  $(2, 0)$  is such an example: if the mama chicken is on square 2 and there are no chicks in the coop, the game will end with at most 7 chicks in the coop. Let  $b_i^R$  be the number of blue squares after square  $i$  on the path and  $b_i^L$  the number of blue squares that come before square  $i$ , including square  $i$ . Note  $b_i^R + b_i^L$  is the total number of blue squares in the game. Then for square  $i$ , the states are  $(i, j)$  with  $\max(i - b_i^R, 0) \leq j \leq \min(i + b_i^L, 8)$ . For example, for square 3,  $b_3^R = 1$  and  $b_3^L = 1$  since there is one blue square to the right of square 3 and one blue square to the left of square 3. Thus square 3 corresponds to possible states  $(3, 2)$ ,  $(3, 3)$ ,  $(3, 4)$ . It is not possible to have more than 4 chicks in the coop on square 3, and if the coop has 0 or 1 chicks on square 3 it is impossible to win the game. All the states are

$$\{(0, 0), (2, 1), (2, 2), (2, 3), (3, 2), (3, 3), (3, 4), (5, 5), (5, 6), (5, 7), (7, 7), (7, 8), \text{win}, \text{loss}\}$$

for this board. For the purposes of building a transition matrix think of  $(0, 0)$  as state 1,  $(2, 1)$  as state 2,  $(2, 2)$  as state 3,  $\dots$ , and “loss” as state 14. Entry  $p_{i,j}$  in the transition matrix for the game is the probability of moving from state  $i$  to state  $j$ . For example, in row 1 of the transition matrix, start in position  $(0, 0)$  on the game board. There is a  $1/3$  probability of rolling a fox; this spin keeps the token in position  $(0, 0)$ , so  $p_{1,1} = 1/3$ . Spinning a sheep is the next possibility, putting the token in position  $(2, 3)$ , or a cow, putting the token in position  $(3, 3)$ . This gives  $p_{1,4} = 1/3$  and  $p_{1,6} = 1/3$ . All other entries in row 1 are 0. Starting in state  $(2, 1)$ , then spinning the sheep puts the token in position  $(7, 6)$ , or the loss state, because if there are only 6 chicks in the coop upon reaching square 7, it is impossible to win. Spinning the fox also puts the game in the loss state, so entry  $p_{2,14} = 2/3$ . Spinning the cow puts the game in state  $(3, 2)$ , so  $p_{2,5} = 1/3$ . All other entries in



[illegible]
$$\begin{pmatrix} Q & R \\ 0 & I \end{pmatrix}$$
[illegible]

Let  $B = NR$ . If the game is in the  $i$ th non-absorbing state then the probability that the game terminates by reaching the  $j$ th absorbing state is  $b_{ij}$ . Then

$$B = \begin{pmatrix} \frac{305}{486} & \frac{181}{486} \\ \frac{5}{81} & \frac{76}{81} \\ \frac{104}{243} & \frac{139}{243} \\ \frac{170}{243} & \frac{73}{243} \\ \frac{5}{27} & \frac{22}{27} \\ \frac{5}{9} & \frac{4}{9} \\ \frac{190}{243} & \frac{53}{243} \\ \frac{5}{9} & \frac{4}{9} \\ \frac{22}{27} & \frac{5}{27} \\ \frac{73}{81} & \frac{8}{81} \\ \frac{2}{3} & \frac{1}{3} \\ \frac{8}{9} & \frac{1}{9} \end{pmatrix}.$$

From the first row of  $B$ , this game has a win probability of  $305/486 \approx 0.6276$  and a loss probability of  $181/486 \approx 0.3724$  when a player begins from the start square. One of the nice aspects of using a Markov chain for these calculations is that a player can update the win probability moving through the game. For example, suppose in two turns the player starts by spinning a sheep and then spins a fox. The coop would first gain 3 chicks, then lose a chick. This state of the game corresponds to the state  $(2, 2)$ , which corresponds to the third row of  $B$ . Therefore in such a situation the player would know that her win probability is now only  $104/243 \approx 0.4280$ .

The computations for the general game are similar except that the matrices  $Q$  and  $R$  are much larger.  $Q$  is  $163 \times 163$  and  $R$  is  $163 \times 2$  and therefore  $B$  is  $163 \times 2$ . It is impractical to enter and compute with such large matrices by hand. The Scripts section has a program to build the matrices and compute the win probability. The matrix  $Q$  in the full game looks similar to the matrix  $Q$  in the small example: the matrix is mostly zeroes punctuated sparsely with small diagonals of entries of value  $1/6$ , instead of  $1/3$ . The top left entry of  $B$  in this case is  $0.6410$ , and the probability of winning a game of *Count Your Chickens!* is  $0.641$ . The length of the game from the start state to absorption in the win or loss states is  $10.83$  moves, with a variance of  $4.43$  moves.

## 7.6. Chapter Ending Answer

The future development of the game at a turn must be independent of the past to model the game as a Markov chain. Games depending on a randomizing device, such as a dice rolls or a spinner, can often be modeled as a Markov chain. Examples in

this section are the games of *Tenzi*, *Chutes and Ladders*, and *Count Your Chickens!*. Strategy games such as checkers or chess are not modeled by Markov chains.

## 7.7. Chapter Summary

### Key Concepts.

- (1) *Tenzi* is a simple dice game for multiple players. The game-play of *Tenzi* for a single player can be modeled with a Markov chain with 10 transient states and 1 absorbing state. Markov chain methods give the distribution of the number of rolls necessary to complete the game, along with the mean and variance.
- (2) The *Towers of Hanoi* is a mathematical game or puzzle. It consists of three rods and some number of disks of different sizes, with holes in the center so each disk can slide onto any rod. The puzzle starts with the disks in a neat stack in ascending order of size on one rod, the smallest at the top, making a conical shape. The objective of the puzzle is to move the entire stack to another rod, obeying 3 rules.
- (3) The children's' game *Chutes and Ladders* is a 100 state Markov chain with a final absorbing state and Markov chain methods give the expected playing time.
- (4) *Count Your Chickens!* is a cooperative counting game for preschoolers. Absorbing Markov chains give the probability of winning a game of *Count Your Chickens!* and the expected number of chicks at the end of the game. The main interest is classifying and counting the states, leading to a  $165 \times 165$  transition probability matrix.

### Vocabulary.

- (1) *Tenzi* is a simple dice game for multiple players.
- (2) The *Towers of Hanoi* is a mathematical game or puzzle. It consists of three rods and some number of disks of different sizes, with holes in the center so each disk can slide onto any rod.
- (3) The children's' game *Chutes and Ladders* is a board game that can be modeled as a 100 state Markov chain with a final absorbing state.
- (4) *Count Your Chickens!* is a cooperative counting board game for preschoolers.

### Notation.

- (1)  $i, j$  – typical states in a game Markov chain
- (2)  $P(j)$  – cumulative probability function for a player getting *Tenzi* on or before the  $j$ th roll
- (3)  $p(j) = P(j) - P(j-1)$  – probability density function for a player getting *Tenzi* on the  $k$ th roll
- (4)

$$P = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix}$$

transition probability matrix is already partitioned

- (5)  $N$  matrix of expected number of rolls a player will spend in each state
- (6)  $m$  – number of disks in Tower of Hanoi problem
- (7)  $aaa, aba, \dots$  – representation of the states for 3
- (8)  $(a, b)$  – A state in *Count Your Chickens!* as an ordered pair where  $a$  is the mama chicken’s position on the board and  $b$  is the number of chicks in the coop
- (9)  $b_i^R$  – the number of blue squares after square  $i$  on the path and
- (10)  $b_i^L$  – the number of blue squares that come before square  $i$ , including square  $i$

## 7.8. Sources

The section on *Tenzi* is adapted from [BP20]. The *Towers of Hanoi* example is adapted from FiveThirtyEight, The Riddler Background information is from Cut The Knot, Towers of Hanoi. Puzzle graphs are examined in more detail in Cut The Knot, Puzzle Graphs The labeling of the states is from Wikipedia, Tower of Hanoi. The reference to the Alekseyev-Berger paper is [AB15]. The section on Chutes and Ladders is adapted from [AKS93]. The section on Count Your Chickens is adapted from [MM19].

## 7.9. Algorithms and Scripts

**Data:** States and transition probabilities for Tenzi  
**Result:** Mean and standard deviation of waiting time to win  
**Result:** Plots of p.d.f. and c.d.f. of waiting time

```

1 Initialization of Matrices
2 Load transition probability matrix
3 for  $i = 2 : 50$  do
4   | Iteratively compute powers of P
5   | Add (1,11) entry to c.d.f. list
6 end
7 Differences of c.d.f. are the p.d.f.
8 Check total probability and approximate mean
9 Extract transient probability submatrix
10 Compute fundamental matrix with matrix inversion
11 Calculate mean from fundamental matrix
12 Calculate variance of waiting times
13 Print mean and standard variation
14 Plot p.d.f. and c.d.f. functions
```

**Algorithm 9:** Tenzi Ladders Game Markov Chain.

**Data:** States and transition probabilities for Chutes and Ladders

**Result:** Mean and standard deviation of waiting time to win

```

1 function rotvec (v)
2   Cyclically rotate vector elements one place to right
3 return rotated vector
4 Initialization of Matrices
5 Load Markov Chain library
6 Set number of states and state names
7 Fill (almost) diceRoll matrix using rotvec
8 Fill diagonal Ladder matrix with moves from ladders
9 Fill diagonal Chutes matrix with moves from chutes
10 Transition probability matrix as product of diceRoll, Ladders, Chutes
    Transition matrix is product of dice roll, ladders and chutes
11 Markov chain calculations
12 Create Chutes and Ladders Markov chain object
13 Compute mean absorption time with library function
14 Extract transient probability submatrix
15 Compute fundamental matrix with matrix inversion
16 Calculate mean from fundamental matrix
17 Calculate variance of waiting times
18 Print mean and standard variation

```

**Algorithm 10:** Chutes and Ladders Game Markov Chain.

**R:** R script for Tenzi.

```

1 x <- c(0.1615055828898457, 0.3230111657796915,
2       0.2907100492017223,
3       0.1550453595742519, 0.05426587585098816,
4       0.01302381020423716,
5       0.002170635034039527, 2.48072575318803*
6       10^-4,
7       1.860544314891023*10^-5, 8.2690858439601*
8       10^-7,
9       1.65381716879202*10^-8, 0.0,
10      0.1938066994678149,
11      0.3488520590420667, 0.2790816472336534,
12      0.1302381020423716,
13      0.03907143061271148, 0.007814286122542296,
14      0.001041904816338973, 8.930612711476907*
15      10^-5,
16      4.465306355738455*10^-6, 9.922903012752121*
17      10^-8, 0.0, 0.0,
18      0.2325680393613778, 0.3721088629782046,
19      0.2604762040847432,
20      0.1041904816338973, 0.02604762040847432,
21      0.004167619265355891,

```

```

12      4.167619265355891*10^-4, 2.381496723060509*
13      10^-5,
14      5.953741807651273*10^-7,0.0, 0.0, 0.0,
15      0.2790816472336534,
16      0.3907143061271148, 0.2344285836762689,
17      0.07814286122542295,
18      0.01562857224508459, 0.001875428669410151,
19      1.250285779606767*10^-4, 3.572245084590763*
20      10^-6,0.0, 0.0,
21      0.0, 0.0, 0.3348979766803841,
22      0.4018775720164609,
23      0.2009387860082305, 0.05358367626886145,
24      0.008037551440329218,
25      6.430041152263375*10^-4, 2.143347050754458*
26      10^-5,0.0, 0.0,
27      0.0, 0.0, 0.0, 0.4018775720164609,
28      0.4018775720164609,
29      0.1607510288065844, 0.03215020576131687,
30      0.003215020576131687,
31      1.286008230452675*10^-4,0.0, 0.0, 0.0, 0.0,
32      0.0, 0.0,
33      0.4822530864197531, 0.3858024691358025,
34      0.1157407407407407,
35      0.0154320987654321, 7.716049382716049*
36      10^-4,0.0, 0.0, 0.0,
37      0.0, 0.0, 0.0, 0.0, 0.5787037037037037,
38      0.3472222222222222,
39      0.06944444444444445,
40      0.004629629629629629,0.0, 0.0, 0.0, 0.0,
41      0.0, 0.0, 0.0, 0.0, 0.6944444444444444,
42      0.2777777777777778,
43      0.02777777777777778,0.0, 0.0, 0.0, 0.0, 0.0,
44      0.0, 0.0, 0.0,
45      0.0, 0.8333333333333334,
46      0.1666666666666667,0.0, 0.0, 0.0,
47      0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0)
48 P <- t( matrix(x, 11, 11) )
49
50 PPow <- P
51 tenzicdf <- c(PPow[1,11])
52 for (i in 2:50) {
53   PPow <- PPow %*% P;
54   tenzicdf <- c(tenzicdf, PPow[1,11])
55 }
56
57 tenzipdf <- tenzicdf[2:50] - tenzicdf[1:49]
58 tenzipdf <- c(tenzicdf[1], tenzipdf)

```

```

42 |
43 | sum(tenzipdf)
44 | tenzimean <- (1:50) %*% tenzipdf
45 |
46 | Q <- P[1:10, 1:10]
47 | I10 <- diag(10)
48 | N <- solve( I10 - Q, I10)
49 |
50 | mean <- N %*% rep(1,10)
51 | Varw <- ((2 * N - I10) %*% N) %*% rep(1, 10) - ( N %
    |   %*% rep(1, 10) )^2
52 | sdw <- sqrt(Varw)
53 | cat("Mean waiting time: ", mean[1], "\nSD of waiting
    |   time:", sdw[1], "\n");
54 |
55 | plot(x = 1:50, tenzicdf, col="red", xlab="Rolls",
    |       ylab="Probability")
56 | points(1:50, tenzicdf, type="l", col="red")
57 | points(1:50, tenzipdf, col="blue")
58 | points(1:50, tenzipdf, type="l", col="blue")

```

**R:** R script for Chutes and Ladders.

```

1 | library("markovchain")
2 |
3 | rotvec <- function(vec) vec[ c(length(vec), 1:(length
    |   (vec)-1)) ]
4 |
5 | nStates <- 100
6 | chutesladdersStates <- as.character( c(1:nStates) )
7 |
8 | diceRoll <- matrix(0, nStates, nStates)
9 | p1 <- c(0,
10 |        1/6, 1/6, 1/6, 1/6, 1/6, 1/6,
11 |        numeric(nStates-7)
12 |        )
13 | for (i in 1:(nStates-5)) {
14 |   diceRoll[i, ] <- p1
15 |   p1 <- rotvec(p1)
16 | }
17 | diceRoll[100, 100] <- 1
18 |
19 | diceRoll[99, 99] <- 5/6; diceRoll[99, 100] <- 1/6
20 |
21 | diceRoll[98, 98] <- 4/6; diceRoll[98, 99] <- 1/6;
    |   diceRoll[98, 100] <- 1/6
22 |

```

```

23 | diceRoll[97, 97] <- 3/6; diceRoll[97, 98] <- 1/6
24 | diceRoll[97, 99] <- 1/6; diceRoll[97, 100] <- 1/6
25 |
26 | diceRoll[96, 96] <- 2/6; diceRoll[96, 97] <- 1/6
27 | diceRoll[96, 98] <- 1/6; diceRoll[96, 99] <- 1/6;
   |   diceRoll[96, 100] <- 1/6
28 |
29 | ladders <- diag(nStates)
30 | ladderIn <- c( 1, 4, 9, 21, 28, 36, 51, 71, 80)
31 | ladderOut <- c(38, 14, 31, 42, 84, 44, 67, 91, 100)
32 | ladders[ cbind(ladderIn, ladderIn) ] <- 0
33 | ladders[ cbind(ladderIn, ladderOut) ] <- 1
34 |
35 | chutes <- diag(nStates)
36 | chuteIn <- c(16, 47, 49, 56, 62, 64, 87, 93, 95, 98)
37 | chuteOut <- c( 6, 26, 11, 53, 19, 60, 24, 73, 75, 78)
38 | chutes[ cbind(chuteIn, chuteIn) ] <- 0
39 | chutes[ cbind(chuteIn, chuteOut) ] <- 1
40 |
41 | chutesladdersMat <- diceRoll %*% ladders %*% chutes
42 |
43 | chutesladders <- new("markovchain", states =
   |   chutesladdersStates, byrow = TRUE,
44 |   transitionMatrix =
   |   chutesladdersMat, name = "ChutesLadders")
45 | meanMC <- meanAbsorptionTime(object=chutesladders)
46 |
47 | Q <- chutesladdersMat[1:99, 1:99]
48 | I99 <- diag(99)
49 | N <- solve( I99 - Q, I99)
50 | absorptionTimeMat <- N %*% rep(1, 99)
51 | meanMat <- mean( absorptionTimeMat[ c(38, 2, 3, 14,
   |   5, 6) ] )
52 | varAbsorptionTimeMat <- ((2 * N - I99) %*% N) %*%
   |   rep(1, 99) - ( N %*% rep(1, 99) )^2
53 | sdAbsorptionTime <- sqrt( mean(
   |   varAbsorptionTimeMat[ c(38, 2, 3, 14, 5, 6) ] ) )
54 |
55 | cat("Mean waiting time from markovchain library: ",
   |   meanMC[1],
56 |   "\nMean waiting time from fundamental matrix: ",
   |   meanMat + 1,
57 |   "\nSD of waiting time:", sdAbsorptionTime[1], "\n");

```

**R:** R script for *Count Your Chickens!*.



```
2 | boardLength <- 40
3 |
4 | animalList <- c("C", "D", "P", "S", "T")
5 | NAnimals <- length(animalList) + 1 # one more for
   |   fox
6 |
7 | blueSquares <- numeric(boardLength)
8 | blueSquares[4] <- 1
9 | blueSquares[8] <- 1
10 | blueSquares[22] <- 1
11 | blueSquares[35] <- 1
12 | blueSquares[39] <- 1
13 |
14 | totalNumberOfBlues <- sum(blueSquares)
15 |
16 | # Setting up the board
17 | board <- character(boardLength)
18 |
19 | board[1] <- "B"
20 | board[2] <- "S"
21 | board[3] <- "P"
22 | board[4] <- "T"
23 | board[5] <- "C"
24 | board[6] <- "D"
25 | board[7] <- "P"
26 | board[8] <- "C"
27 | board[9] <- "D"
28 | board[10] <- "S"
29 | board[11] <- "T"
30 | board[12] <- "B"
31 | board[13] <- "C"
32 | board[14] <- "P"
33 | board[15] <- "B"
34 | board[16] <- "B"
35 | board[17] <- "B"
36 | board[18] <- "T"
37 | board[19] <- "B"
38 | board[20] <- "T"
39 | board[21] <- "D"
40 | board[22] <- "S"
41 | board[23] <- "C"
42 | board[24] <- "D"
43 | board[25] <- "P"
44 | board[26] <- "T"
45 | board[27] <- "B"
46 | board[28] <- "S"
47 | board[29] <- "C"
```

```

48 board[30] <- "B"
49 board[31] <- "B"
50 board[32] <- "T"
51 board[33] <- "P"
52 board[34] <- "S"
53 board[35] <- "D"
54 board[36] <- "B"
55 board[37] <- "S"
56 board[38] <- "C"
57 board[39] <- "P"
58 board[40] <- "CDPST"
59
60 # Count how many states
61 statesIndex <- 1 #initial state (0,0)
62 statesCount <- 1
63 statesHolder <- matrix(0, boardLength *
    totalNumberOfBlues, 2)
64
65 for (i in 1:(boardLength - 1)) {
66     # don't use last space, the 'coop'
67     if (board[i] != "B") {
68         bLi <- sum(blueSquares[1:i]) #blueSquares to
        Left of i, including i
69         bRi <- sum(blueSquares[(i + 1):boardLength])
        #blueSquares to Right of i
70
71         maxChickens <- min(boardLength, i + bLi)
72         minChickens <- max(0, i - bRi)
73
74         statesCount <- statesCount + maxChickens -
        minChickens + 1
75         for (j in minChickens:maxChickens) {
76             statesIndex <- statesIndex + 1
77             statesHolder[statesIndex, ] <- c(i, j)
78         }
79     }
80 }
81 statesHolder[statesCount + 1, ] <- c(Inf, Inf) # win
    state
82 statesHolder[statesCount + 2, ] <- c(-Inf, -Inf) #
    lose state
83 statesCount <- statesCount + 2 #add final won and
    loss states
84 states <- statesHolder[1:statesCount, ]
85 rm(statesHolder)
86
87 Q <- matrix(0, statesCount - 2, statesCount - 2)

```

```

88 R <- matrix(0, statesCount - 2, 2)
89 I <- diag(2)
90 Z <- matrix(0, 2, statesCount - 2)
91
92 for (i in 1:(statesCount - 2)) {
93   currentSquare <- states[i, 1]
94   chicksInCoop <- states[i, 2]
95   currentState <- i
96
97   # This sets transition probabilities from
98   # spinning a fox
99   if (chicksInCoop == 0) {
100     Q[i, i] <- 1/NAnimals # stay in current
101     state, prob 1/NAnimals
102   } else if (states[i - 1, 1] == currentSquare) {
103     Q[i, i - 1] <- 1/NAnimals # remove 1 chick,
104     fill trans prob
105   } else {
106     # too few chicks, must lose
107     R[i, 2] <- R[i, 2] + 1/NAnimals # so add to
108     lose probability
109   }
110
111   # Now set transition probabilities from other
112   # five animals.
113   for (animal in animalList) {
114
115     nextSquare <- grep(animal, board[(
116     currentSquare + 1):boardLength])[1] +
117     currentSquare
118
119     if (blueSquares[nextSquare] == 0) {
120       # not Blue, just add advance
121       updatedChicksInCoop <- chicksInCoop + (
122       nextSquare - currentSquare)
123       if (updatedChicksInCoop > boardLength)
124         updatedChicksInCoop <- boardLength
125     } else {
126       # Blue square, so add extra chick
127       updatedChicksInCoop <- chicksInCoop + (
128       nextSquare - currentSquare) +
129       1
130       if (updatedChicksInCoop > boardLength)
131         updatedChicksInCoop <- boardLength
132     }
133
134     in_states <- FALSE

```

```

126
127     for (p in 1:statesCount) {
128         if (states[p, 1] == nextSquare && states[
p, 2] == updatedChicksInCoop) {
129             in_states <- TRUE
130             newLocation <- p
131             break
132         }
133     }
134
135     if (in_states == TRUE) {
136         Q[i, newLocation] <- 1/NAnimals
137     } else {
138         if (nextSquare == boardLength &&
updatedChicksInCoop == boardLength)
139         {
140             R[i, 1] <- R[i, 1] + 1/NAnimals
141         } # win
142     else {
143         R[i, 2] <- R[i, 2] + 1/NAnimals #
lose
144     }
145 }
146 }
147 }
148
149 # Calculate win-lose probabilities with fundamental
matrix: (I-Q)^{-1} R
150 IsC <- diag(statesCount - 2)
151 matrixProbs <- solve(IsC - Q, R)

```

## 7.10. Problems to Work for Understanding

Chapter 7: Games.

7.1: Write a script in some computer language to replicate the calculations and graphs for the Markov chain for *Tenzi*.

7.2: The c.d.f. and p.d.f. functions  $P(j)$  and  $p(j)$  above respectively summarize the probability that a single player will get Tenzi in  $j$  rolls. What if  $n$  people are playing? This essentially taking  $n$  independent random samples from the probability distribution  $p(j)$ , and identifying the minimum value(s) of  $j$  as the roll in which the game is won. For example, if there are  $n = 5$  players, take 5 independent random samples from  $p(j)$ . Suppose the arbitrary values of  $j$  are [12, 20, 15, 9, 28], representing the number of rolls needed for each player to get Tenzi. Then the 4th player wins the game in 9 rolls.

- (1) In general, write an expression for the probability that the minimum value from  $n$  random samples of  $p(j)$  is less than or equal to  $j$  in terms of  $P(j)$ .
  - (2) Using the probability distributions from the scripts find the expected number of turns in a game of Tenzi with 2, 3 and 4 players.
- 7.3: Show that the shortest possible game of *Chutes and Ladders* consists of 7 moves by listing those moves.
- 7.4: Consider the effect of chutes and ladders on the waiting time to absorption.
- (a) Find the expected waiting time to absorption in a game with no chutes or ladders.
  - (b) In the original game, insert an additional ladder from state 46 to state 94. What happens to the expected waiting time?
  - (c) In the original game, instead insert a chute from state 83 to state 7. What happens to the expected waiting time?
  - (d) Add a ladder to the original game from state 79 to state 81. What happens to the expected waiting time?
  - (e) Add a chute to the original game from state 29 to state 27. What happens to the expected waiting time?
- 7.5: Investigate the following modifications to the small *Count Your Chickens!* game.
- (a) What is the win probability if only square 2 is blue? What is the win probability if squares 2, 3 and 5 are blue?
  - (b) What effect does adding additional animals to the board (i.e., increasing the size of the spinner) have?
  - (c) What if the fox removes more than one chick from the coop?
  - (d) What effect does changing the size of each character's space in the spinner do? For example, what if the fox covered  $1/3$  of the spinner and the remaining five animals each took up  $2/15$  of the spinner?
  - (e) What if some of the blue squares were colored green and had the effect of moving an additional two chicks into the coop?
  - (f) Create your own questions that can be analyzed using Markov chains and to modify the supplemental R code to answer the questions.
- 7.6: Assume Alice and Bob toss a fair coin. In each toss head (H) or tail (T) can show up with equal probability.
- Alice and Bob choose some sequence of H and T they are waiting for. Assume that the chosen sequences have equal length  $n$  and are different. For example for  $n = 3$  Alice could choose THH and Bob HHT. The winner of the game is the person who sees their sequence first.
- (1) Suppose  $n = 2$  and Alice chooses TH and Bob chooses HH. Who is more likely to win?
  - (2) Suppose  $n = 3$  and Alice chooses THH and Bob chooses HHH. Who is more likely to win?
  - (3) Suppose  $n = 3$  and consider all possible preferred sequences of Alice and Bob and create a graph that keeps track of which sequences beat other sequences.
  - (4) For  $n = 3$  can *winning dominance cycles* exist? That is, that is, for example, that sequence  $s_1$  beats  $s_2$ ,  $s_2$  beats  $s_3$ , and  $s_3$  beats  $s_1$ ?

(5) For  $n = 4$  can *winning dominance cycles* exist?

7.7: You are going to play a game. Like many probability games, this involves an infinite supply of ping-pong balls labeled with integers. The balls are numbered 1 through  $N$ , so there are infinitely many labeled 1, infinitely many labeled 2, and so on up to  $N$ . There is also a group of  $N$  cups, labeled 1 through  $N$ , each of which can hold an unlimited number of ping-pong balls. The game is played in rounds. A round is composed of 2 phases: throwing and pruning.

During the throwing phase, the player takes balls randomly, 1 at a time, from the supply and tosses them at the cups. The throwing phase is over when every cup contains at least 1 ping-pong ball. Next comes the pruning phase. During this phase the player goes through all the balls in each cup and removes any ball whose number does not match the containing cup.

Every ball drawn has a uniformly random number from 1 to  $N$ , every ball lands in a uniformly random cup, and every throw lands in some cup. The game is over when, after a round is completed, there are no empty cups.

- (a) How many balls would you expect to need to draw and throw to finish this game?
- (b) For  $N = 3$ , how many rounds would you expect to need to play to finish this game?



## Modeling Baseball as a Markov Chain

This chapter assumes familiarity with the rules and terminology of American baseball and some of the statistics associated with baseball players. The goal is to model a half-inning of a baseball game as a relatively simple Markov chain to find the expected number of runs a player will score as a means of evaluating and comparing players. A secondary goal is to propose a simple Markov chain as a basis for more detailed and realistic models of the game of baseball.

Mathematically Mature: contains mathematics beyond calculus with proofs.

### 8.1. Chapter Starter Question

What is the baseball statistic known as *OPS*? How is this statistic used?

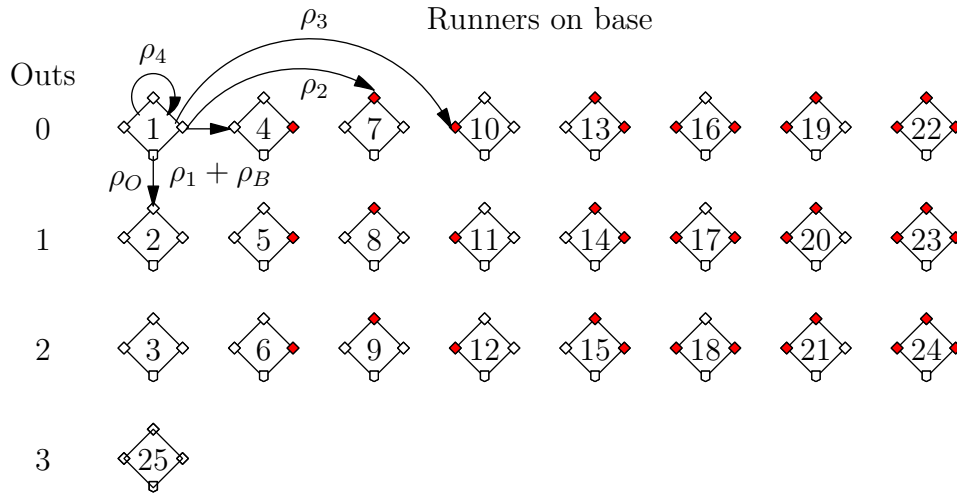
### 8.2. States and Transition Probability Matrix

The Markov chain will be the sequence of situations arising in a half-inning of a baseball game. In this Markov chain model of baseball each step will be a plate appearance. A plate appearance is similar to an at-bat, but includes walks, hit batters, and sacrifices that recorded baseball does not regard as an official at-bat. In this baseball model, the states are the runners on base together with a count of the present outs. Each plate appearance has eight possibilities for the runners on base:

- the bases can be empty;
- there can be one runner on first, second, or third base;
- there can be two runners on base in three different ways; or
- the bases can be loaded.



Runners:	None	1st	2nd	3rd	1&2	1&3	2&3	1,2,&3
Outs								
0	1	4	7	10	13	16	19	22
1	2	5	8	11	14	17	20	23
2	3	6	9	12	15	18	21	24
3	25							

**Table 8.1.** States of the Markov chain model of a half inning of baseball**Figure 8.1.** The state diagram for the Markov chain model of a half-inning of baseball, with only transitions from state 1 indicated as an example.

The number of outs can be 0, 1, or 2 to make twenty-four states. All situations with three outs are the same, and this situation is the final 25th absorbing state. Once the game reaches this state, the half-inning ends and the Markov chain is stopped. This simplified model takes no account of how many players are on base or where players are located when the third out is made. Table 8.1 gives the labeling of the 24 possible runners and outs states. Figure 8.1 is a diagram of the states along with a few sample transitions. The model tracks runs scored separately, runs are not part of the states. Osbourne *et al.* [OWD20], use the same set of states with more descriptive state labels but ordering them left to right in a row, then row by row.

Denote the probability of moving from one state  $i$  to state  $j$  by  $p_{i,j}$ . Many transitions are impossible, such as a transition to a state with fewer outs, and hence have probabilities equal to zero. Using the numbering above,  $p_{1,4}$  is the probability of going from no outs and no runners on base to a runner on first with no outs, which in turn is equal to the probability of a single plus the probability of a walk. In real baseball, there are other possibilities for this transition such as a wild pitch, but this simplified model ignores them. In certain situations different actions by the batter produce the same effect. As can be seen in Figure 8.1, if no

one is on base, then a single and a walk have the same effect. Sum the probability of each event to give the state transition probability.

For this model imagine that the player bats with plate outcomes distributed randomly according to his statistical profile. Plate appearances are independent. In other words, a player's chance of getting a specific kind of hit or making a specific kind of out is independent of how many runners are on and the number of outs. Based on this profile, compute the transition probabilities for each pair of states, obtaining the transition matrix. The transition probabilities could come from player statistics from the previous year, the current year, or the career, but must use the same profile each time. The transition probability matrix  $P$ , whose entries are  $p_{i,j}$  governs the evolution of the half inning. By the properties of matrix multiplication,  $P^2$  is the transition matrix for sequences of two plays or batters,  $P^3$  is the transition matrix for sequences of three batters, and so on, for a string of identical batters. This assumption is useful for computing *average* performance which is the goal here, but not for specific game situations.

### 8.3. Assumptions of the Model

Encoding the half inning of the game in the transition matrix like this requires simplifying assumptions.

- (1) The Markov property assumption means that this model does not take into account how it arrived at a particular situation. For example, if there is a runner on first and no outs, the Markov chain model is not concerned about whether there was a walk or a single.
- (2) More specifically, the Markov property assumption deliberately eliminates the possibility of a *clutch hitter*. Such a player allegedly hits better when the situation matters more, but numerical studies indicate that the concept is an illusion.
- (3) A related question is whether players get "hot" or "cold", the model ignores this possibility.
- (4) This model ignores situations such as stolen bases or pick-offs that could occur during the plate appearance, changing the state without action from the player in his plate appearance.
- (5) The model ignores double plays, sacrifice bunts, and sacrifice flies.
- (6) The model ignores runs scored while incurring the third out.
- (7) An important simplifying assumption is that the matrix is time independent, and each plate appearance is an independent event. In real baseball, as pitchers and batters face each other multiple times, each adjusts to the other, changing the probabilities. Fatigue may also be a factor as a game progresses.
- (8) Another related assumption is that the batter's outcomes do not depend on the pitcher and what the pitcher does is not dependent on the hitter. The probabilities remain constant, regardless of the current match-up and previous encounters between pitcher and hitter.
- (9) The model assumes that a single advances runners already on base by two bases. For example, in states 4, 5, or 6 with runner on first, a single by the

hitter moves the base runner to third base, leaving the chain in states 16, 17, or 18 respectively. Also, assume that a double advances each runner two bases, so that in states 4, 5, or 6 with runner on first, a double by the hitter moves the base runner to third base, leaving the chain in states 19, 20, or 21. In contrast, in [CK77] Cover and Keilers explicitly make the assumption that “All singles and doubles are assumed to be long. That is, a single advances a baserunner two bases, and a double scores a runner from first base.” On the other hand, Pankin [Pan] is not explicit about this assumption, but Markov chain simulations imply that more detailed base running plays have nonzero probability. For instance, Pankin implies the possibility that bases loaded with one out (state 23) can change to state 5 or 8 meaning that a runner on first, as well as the two runners on second and third, can score on a single or a double. Likewise Pankin implies that a change from state 23 to 23 is possible which would be a single allowing one run from third, advancing the runners on first and second one base. As another example, Osbourne *et al.* [OWD20] show how to estimate the probabilities that with no outs and a baserunner on first, after a single the baserunner advances to second or third, or even scores all the way from first. The simpler Markov chain model here does not assume these additional baserunning and scoring refinements.

- (10) Bukiet *et al.* [BHP97] present an algorithm to carry Markov calculations for one inning forward across a full game, keeping track of the probability distribution of runs scored, instead of just a half-inning considered here.

Each assumption can be relaxed at the cost of more states and a larger transition probability matrix, or using more detailed player statistics or both. For example, Osbourne *et al.* [OWD20] show how to estimate the probability of a sacrifice fly or grounding into a double play. However they specifically neglect events such as a four-base error (a rare event where a fielder’s error allows a hitter to round the bases to score) in transition  $P_{1,1}$ , or reaching base by error, or by hit-by-pitch, also ignored here. The intent here is to show how to model baseball as a relatively simple Markov chain, in the process creating a new player evaluation statistic.

#### 8.4. Player Statistics

A particular batter  $H$  determines a twenty-five by twenty-five matrix  $P$  from his statistical profile. For convenience, write the player’s profile as follows, deviating slightly from the standard listing. Here  $AB$  denotes at-bats,  $S$  denotes singles,  $D$  denotes doubles,  $T$  denotes triples,  $HR$  denotes home runs,  $BB$  denotes walks plus hit batters,  $AVE$  denotes batting average  $(S+D+T+HR)/AB$ ,  $SA$  denotes slugging average  $(1 \cdot S + 2 \cdot D + 3 \cdot T + 4 \cdot HR)/AB$ , a measure of the batting productivity of a player,  $OB$  denotes on-base average  $(BB + S + D + T + HR)/(AB + BB)$ , and  $OPS = OB + SA$  measuring the ability of a player both to get on base and to hit for power, two important offensive skills. Note that the last four columns in 8.2 derive from the first six, and hence are not actually needed. For this model, the number of plate appearances is  $AB + BB$ , ignoring sacrifice flies as in the official score-keeping. In this simplified scenario, all outs are equivalent, there is no practical difference between a strikeout and a pop-out. As a result, values of  $OB$  and  $OPS$  here differ slightly from the official records. These statistics give the complete profile of  $H$  for

	<i>AB</i>	<i>S</i>	<i>D</i>	<i>T</i>	<i>HR</i>	<i>BB</i>	<i>AVE</i>	<i>SA</i>	<i>OB</i>	<i>OPS</i>
X	500	100	25	5	30	100	.320	.570	.433	1.003
MT M	470	63	27	2	45	110	.291	.645	.426	1.071
CB	558	86	34	3	47	95	.305	.629	.406	1.035
AJ	559	85	36	1	58	133	.322	.701	.458	1.159
SO	636	98	38	7	54	81	.310	.436	.646	1.036

**Table 8.2.** Statistics for representative players.

the model. In other words, the player statistics determine the probabilities that H makes each kind of hit or out, draws a walk, gets hit by a pitch, and so on.

For example, Table 8.2 gives a fictional line for a hypothetical star player X. Table 8.2 also includes season profiles for Mike Trout (Los Angeles Angels, American League MVP for 2019), Cody Bellinger (Los Angeles Dodgers, National League MVP for 2019), Aaron Judge (New York Yankees, American League MVP for 2024), and Shohei Ohtani (Los Angeles Dodgers, National League MVP for 2024) as examples of recent player statistics. Player X has 500 at-bats but 600 plate appearances. In a given plate appearance player X has a  $\frac{1}{6}$  chance to hit a single, a  $\frac{1}{6}$  chance to reach first base by a walk or hit batter, a  $\frac{1}{120}$  chance to hit a triple, and so on. In this way, from the 6 basic player statistics, compute a probability distribution  $(\rho_O, \rho_B, \rho_1, \rho_2, \rho_3, \rho_4)$ , where  $\rho_O$  is the probability of an out,  $\rho_B$  is the probability of a base on balls, and  $\rho_i$  is the probability of an  $i$ -base hit.

## 8.5. Constructing the Transition Probability Matrix

A state can change in several ways, for instance state 16 with runners on first and third with no outs can change into state

- 17 with an out,
- 22 with a base on balls advancing the runner on first,
- 16 back to itself while scoring a run with a single,
- 19 with a double scoring both base runners,
- 10 with a triple, or
- 1 with a home run.

A convenient way to build the transition probability matrix is to compose it from 6 simpler matrices with entries either 0 or  $\rho_x$ , corresponding to the 6 probabilities in the hitter's distribution. For example, for  $\rho_O$ , the probability of an out, the number of outs increases by one and the base runners remain the same, which makes a regularly shaped transition matrix  $P_0$ , where states with an index divisible by 3 transition to the absorbing state 25 of three outs. All other states advance by 1 index with probability  $\rho_O$ . Taking  $P_3$  as another example, a triple scores all runners already on base, leaves the hitter on third base and the numbers of outs stays the same. Thus in  $P_3$  each state transitions to state 10, 11 or 12 according to the existing number of outs. The other 4 matrices are similar, but the advance of states is slightly more complicated because of the assumption that runners on base

advance by 2 bases on a hit. Finally, the full transition probability matrix is the sum of the 6 elementary transition matrices:  $P = P_O + P_B + P_1 + P_2 + P_3 + P_4$ . Set  $P_{25,25} = 1$  to account for the absorbing end state. The transition probability matrices are too large to display here, but the scripts below build the matrices given the values for  $(\rho_O, \rho_B, \rho_1, \rho_2, \rho_3, \rho_4)$ .

Keeping track of runs scored will be an important outcome of the model. The new statistic called *Markov runs* is how many runs a team could score by using this player for every plate appearance. The complete definition follows. Cover and Keilers [CK77] call this the *Offensive Earned-Run Average* or OREA but that term seems to be no longer used. This statistic, normalized using nine innings, for all players each day of the season is available at Sagarin ratings labeled as “markov RPG” (Runs Per Game). Given the player’s statistical profile, the player bats according to the Markov chain model until making three outs. In principle the test is run thousands of times, and from it the model determines the average number of runs scored per nine innings. However, simple results from Markov chain theory calculate the statistics without needing thousands of simulations.

## 8.6. Calculating Markov Runs

Let  $R$  be the  $25 \times 1$  column vector containing the expected or average runs scored after each state on one play only. Denoting the elements of  $R$  by  $R_1, R_2, \dots, R_{25}$  some example calculations are:

$$\begin{aligned} R_1 &= p_{1,1} \text{ (based on a home run)} \\ R_2 &= p_{2,2} \text{ (based on a home run)} \\ R_6 &= p_{6,12} + 2p_{6,3} \text{ (based on triple or a home run)} \\ R_{17} &= p_{17,17} + p_{17,20} + 2p_{17,11} + 3p_{17,1} \\ R_{23} &= 2p_{23,17} + 2p_{23,20} + 3p_{23,11} + 4p_{23,2} \\ R_{25} &= 0. \end{aligned}$$

The vector of runs calculated here will be componentwise slightly less than the run vector for Cover and Keilers because advances on singles and doubles are less than they assume. Likewise, the vector of runs calculated here will be componentwise less than the run vector for Pankin because some state transitions he considers are ignored here.

The key output of the Markov chain baseball model is the computation of the expected runs in the rest of the inning after any runners and outs state. Let  $E$  be the  $25 \times 1$  column vector containing these values. Then,

$$E = R + PR + P^2R + P^3R + \dots$$

This equation says that the expected runs after any state is the sum of the expected runs after one plate appearance, the expected runs after two plate appearances, and so on theoretically forever. Of course, almost surely (in the probability sense!) the half-inning will end sometime in the 25th absorption state of three outs. Because the vector of runs calculated here is less than the other run vectors, the expected run vector, or Markov runs will be slightly less. Since the 25th state with 3 outs is the

only absorbing state and the other 24 states are transient, the  $25 \times 25$  probability transition matrix partitions into the block matrix

$$P = \begin{pmatrix} Q & Q' \\ 0 & 1 \end{pmatrix}$$

where  $Q$  is  $24 \times 24$ , and  $Q'$  is  $24 \times 1$ . This block matrix has the typical form for games because it is natural to order the absorbing state as the last state 25. Since no runs are scored from the 25th absorbing state, just consider

$$E' = R' + QR' + Q^2R' + Q^3R' + \dots$$

where  $R'$  and  $E'$  are the  $24 \times 1$  subvectors of  $E$  and  $R$  corresponding to the first 24 entries. By standard matrix theory, this is equal to

$$E' = (I_{24} - Q)^{-1} R'.$$

The expected runs vector  $E'$  has useful interpretations. For example, if  $P$  uses statistics for all events for a league, then  $E'$  contains the league average expected runs scored in the rest of the inning from each runners-and-outs state. With enough statistics, similar values for teams, a team's home and road games, or for an individual player can be calculated. The last case for an individual player is the per inning estimate of run scoring if that player batted all the time. Another application would be restricting the transitions to those not influenced by strategies such as stolen bases or sacrifice bunts. Then the expected run values of games without stolen bases or sacrifice bunts can be compared to games using those strategies.

Note that  $E'_1$  is the expected runs after the no-runners-no-outs state in which all innings begin. Thus **Markov runs per game**  $9E'_1$  is the expected number of runs per 9 half-innings, or per game. This computation is especially interesting when applied to an individual player's statistics. The value for the mythical player X is 9.49. This statistics provides another way of estimating how many runs per game a player would score by batting all the time. As noted above, some baseball statisticians report this number for players, but much more common is the **On-base plus slugging** statistic or *OPS*. For *OPS*, simply add the player's slugging average to his on-base average. This simply computed player statistic empirically correlates fairly well with the expected number of runs scored using the Markov chain model. More details are in the article by D'Angelo [D'A10].

## 8.7. Changes to the Model

The elementary model here assumes a series of identical batters, of course this does not happen in real games. This has been the major criticism of the applicability of Markov models. But it is possible to have a Markov model with different transition matrices for each batter, see [OWD20] for an example. Then the assumption of stationarity is dropped and the transition probability matrix changes with each batter according to that batter's statistics. Instead of powers of one transition matrix  $P$ , use products of the matrices for each batter:  $P_1P_2$ ,  $P_1P_2P_3$ , etc. Also, the expected runs on the next play column vector  $R$  has to be modified for each batter. With such changes, the expected runs generalizes to

$$E = R_1 + P_1R_2 + P_1P_2R_3 + P_1P_2P_3R_4 + \dots$$

An additional potential complication is that it may be necessary to repeat the calculation for several sequences with different first batters and then weight the results by the probability of specific batters beginning the sequence. The model can be expanded in a number of ways and the utility is limited only by the amount of data available.

## 8.8. Chapter Ending Answer

*OPS* is the sum of “on-base percentage” and “slugging percentage” to get one number that unites the two. *OPS* is meant to combine how well a hitter can reach base with how well he can hit for average and for power. “On-base percentage” refers to how frequently a batter reaches base per plate appearance. Times on base include hits, walks and hit-by-pitches, but do not include errors, times reached on a fielder’s choice or a dropped third strike. “Slugging percentage” represents the total number of bases a player records per at-bat.

## 8.9. Chapter Summary

### Key Concepts.

- (1) The goal is to model a half-inning of a baseball game as a Markov chain to find the expected number of runs a player will score as a means of evaluating and comparing players.
- (2) The expected number of runs a player will score uses the standard partition of the transition probability matrix over the transient and absorbing states.
- (3) A convenient way to build the transition probability matrix is to compose it from 6 simpler matrices with entries either 0 or  $\rho_x$ , corresponding to the 6 probabilities in the hitter’s distribution.

### Vocabulary.

- (1) A new baseball statistic is how many runs will a team score if it uses a player for every plate appearance, called **Markov runs**.
- (2) The **On-base plus slugging** statistic or *OPS* is the sum of a player’s slugging average and his on-base average.

### Notation.

- (1)  $p_{i,j}$  – the probability of moving from one state  $i$  to state  $j$
- (2)  $AB$  denotes at-bats,  $S$  denotes singles,  $D$  denotes doubles,  $T$  denotes triples,  $HR$  denotes home runs,  $BB$  denotes walks plus hit batters,  $AVE$  denotes batting average  $(S + D + T + HR)/AB$ ,  $SA$  denotes slugging average  $(1 \cdot S + 2 \cdot D + 3 \cdot T + 4 \cdot HR)/AB$ , a measure of the batting productivity of a player,  $OB$  denotes on-base average  $(BB + S + D + T + HR)/(AB + BB)$ , and  $OPS = OB + SA$  measuring the ability of a player both to get on base and to hit for power
- (3)  $(\rho_O, \rho_B, \rho_1, \rho_2, \rho_3, \rho_4)$  – probability distribution where  $\rho_O$  is the probability of an out,  $\rho_B$  is the probability of a base on balls, and  $\rho_i$  is the probability of an  $i$ -base hit.

- (4)  $R$  – the  $25 \times 1$  column vector containing the expected or average runs scored after each state on one play only. The elements of  $R$  are  $R_1, R_2, \dots, R_{25}$
- (5)  $E$  – the expected runs in the rest of the inning after any runners and outs state
- (6)  $Q, Q'$  – submatrices of the transition probability matrix corresponding to transitions among the transients and the transients to the stationary state.  $E'$  corresponding expected runs subvector.
- (7)  $I_{24}$  –  $24 \times 24$  identity matrix.

### 8.10. Sources

This section is adapted from the articles [CK77, D'A10, OWD20] and [Pan]. Each of those articles has many further references. The online article The Markov Chain Model of Baseball has the same basic information as this article, but in a condensed form. The definition of *OPS* is adapted from On-base Plus Slugging

### 8.11. Algorithms and Scripts

**Data:** Basic player statistics

**Result:** Markov runs from each state for the player

- 1 *Initialization*
- 2 Enter player statistics
- 3 Initialize with zero simple matrices for the player statistics
- 4 Fill simple matrices with corresponding player statistic
- 5 Transition probability matrix is sum of simple matrices
- 6 Create runs scored matrix
- 7 Expected runs as product of runs scored matrix with player statistics
- 8 *Calculation of Markov runs*
- 9 Direct matrix calculation of Markov runs from submatrix
- 10 Load markovchain library and initialize
- 11 Calculate Markov runs as expectedRewards()
- 12 **return** *Markov runs from each state*

**Algorithm 11:** Markov chain simulation.

```

1 # Player X Statistics
2 rho0 <- 340/(500 + 100)
3 rhoB <- 100/(500 + 100)
4 rho1 <- 100/(500 + 100)
5 rho2 <- 25/(500 + 100)
6 rho3 <- 5/(500 + 100)
7 rho4 <- 30/(500 + 100)
8
9 P0 <- matrix(0, nrow=25, ncol=25)
10 PB <- matrix(0, nrow=25, ncol=25)
11 P1 <- matrix(0, nrow=25, ncol=25)
12 P2 <- matrix(0, nrow=25, ncol=25)

```



```

13 P3 <- matrix(0, nrow=25, ncol=25)
14 P4 <- matrix(0, nrow=25, ncol=25)
15
16 ## State      1    2    3    4    5    6    7    8    9    10
17      11  12  13  14  15  16  17  18  19  20  21  22  23
18      24
19 transitionOut <- c(2, 3, 25, 5, 6, 25, 8, 9, 25, 11,
20                    12, 25, 14, 15, 25, 17, 18, 25, 20, 21, 25, 23, 24,
21                    25)
22 transitionBB  <- c(4, 5, 6, 13, 14, 15, 13, 14, 15, 16,
23                    17, 18, 22, 23, 24, 22, 23, 24, 22, 23, 24, 22, 23,
24                    24)
25 transition1B  <- c(4, 5, 6, 16, 17, 18, 4, 5, 6, 4,
26                    5, 6, 16, 17, 18, 16, 17, 18, 4, 5, 6, 16, 17,
27                    18)
28 transition2B  <- c(7, 8, 9, 19, 20, 21, 7, 8, 9, 7,
29                    8, 9, 19, 20, 21, 19, 20, 21, 7, 8, 9, 19, 20,
30                    21)
31 transition3B  <- c(10, 11, 12, 10, 11, 12, 10, 11, 12,
32                    10, 11, 12, 10, 11, 12, 10, 11, 12, 10, 11, 12, 10,
33                    11, 12)
34 transitionHR  <- c(1, 2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3, 1,
35                    2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3)
36
37 for (i in 1:24) {
38   P0[i, transitionOut[i]] <- rho0
39   PB[i, transitionBB[i]]  <- rhoB
40   P1[i, transition1B[i]]  <- rho1
41   P2[i, transition2B[i]]  <- rho2
42   P3[i, transition3B[i]]  <- rho3
43   P4[i, transitionHR[i]]  <- rho4
44 }
45
46 P <- P0 + PB + P1 + P2 + P3 + P4
47 P[25, 25] = 1
48
49 M <- matrix(0, nrow=25, ncol=5)
50 M[22:24, 1] <- 1
51 M[7:18, 2:3] <- 1
52 M[19:24, 2:3] <- 2
53 M[4:12, 4] <- 1
54 M[13:21, 4] <- 2
55 M[22:24, 4] <- 3
56 M[1:3, 5] <- 1
57 M[4:12, 5] <- 2
58 M[13:21, 5] <- 3
59 M[22:24, 5] <- 4

```

```

47 playerX <- c(rhoB, rho1, rho2, rho3, rho4)
48 runsX <- M %*% playerX
49
50
51 Q <- P[1:24, 1:24]
52 cat( solve(diag(24) - Q, runs[X1:24]) )
53 cat(' '\n\n')
54
55 library("markovchain")
56 nStates <- 25
57 baseballStates <- as.character(c(1:nStates))
58 mcBaseball <- new("markovchain", states = baseballStates,
59   byrow=TRUE, transitionMatrix = P, name="mcX")
60 cat( expectedRewards(mcBaseball, 30, runX) )

```

## 8.12. Problems to Work for Understanding

Chapter 8: A Markov Chain Model of Baseball.

8.1: Steven Strasburg of the Washington Nationals was the 2019 World Series MVP. Discuss why this model may not be useful for assessing Strasburg as a baseball player.

8.2: With this model, what is the expected number of at-bats for (9 copies of) Mike Trout until the third out in a half-inning?

8.3: Consider a player  $K$  who each time at bat either hits a home run with probability  $q$  or strikes out with probability  $1 - q$ . Write out the nonzero transition probabilities in the matrix  $P_K$ .

8.4: Find the player statistics for the MVP in the National League and American League for the previous complete baseball season and compute the Markov runs for each.

8.5: Use this model to calculate the Markov runs for Ted Williams and Babe Ruth. Does this settle the debate about who is the greatest hitter in baseball history?



## Modeling Sports With Markov Chains

Tennis and basketball are modeled with Markov chains with 20 and 8 states respectively. For tennis, winning or losing are absorbing states of the Markov chain. For basketball, the sample path of the chain provides a score for the game. These two familiar sports illustrate previously derived methods for Markov chains.

Student: contains scenes of mild algebra or calculus that may require guidance.

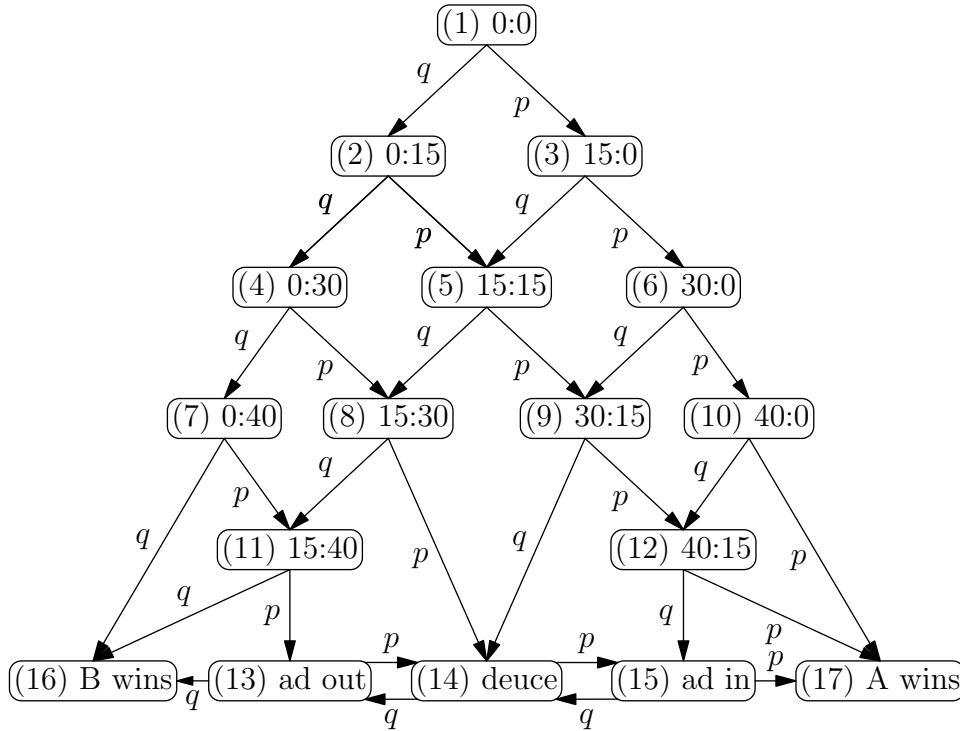
### 9.1. Chapter Starter Question

What is your favorite sport? Does the sport have discrete “states” that can be modeled with a Markov chain? What sports analytic measures exist to measure the game?

### 9.2. Tennis

Tennis is a popular sport played as a sequence of “games” making up a “set” and several sets making a “match”, determining the overall winner. One player in a game is the server, and the opposing player is the receiver. A coin toss determines the server in the first game. Service alternates game by game between the two players or teams.

A tennis game consists of a sequence of points played with the same player serving. The first player to gain 4 points in total and at least two points more than the opponent wins. The scoring of tennis is unusual for historical reasons that are not clear. Roughly speaking, a player’s point score advances by 15 when a player scores because the opponent missed returning the ball or hits it out of bounds, with a few more technical rules. The maximum score to win a game is 60 so game scores should be 0, 15, 30, 45, and 60. But tradition abbreviates the third score to 40, and calls the 0 score “love” for reasons that are again historically unclear.



**Figure 9.1.** The state transition diagram for a game of tennis. The score for player A is first, separated by a colon from the score for player B. The numbers in parentheses are the row and column numbers of the state in the transition probability matrix. The probability labels are the same as the analogous random walk probabilities.

Thus, the running score of each game is special to tennis: scores from zero to three points are “love”, “15”, “30”, and “40”, respectively. If each player has at least three points, making the player’s scores equal at 40, the score is not called out as “40–40”, but rather as “deuce”. If at least three points have been scored by each side and a player has one more point than the opponent, called “ad in” when the serving player is ahead, and “ad out” when the receiving player is ahead.

To model tennis as a Markov chain, take the states of the chain as the possible scores for the two players. For simplicity, assume that transition from one state or score to another is constant and depends only on the present score and not on the preceding states or scores. Figure 9.1 illustrates the transitions among the states. Clearly this assumption is idealizing the game, leaving out factors such as the order of service, psychological factors, fatigue, or adaptation to the opponent’s style. Other factors not mentioned can also affect the transition probabilities.

As is natural for a game or a sport, this Markov chain has two absorbing states, “A wins” and “B wins”. Because the victor of the game must win by at least 2 points, after 4 or 5 transitions the final set of states “B wins”, “30:40”, “30:30”, “40:30”, “A wins” creates an absorbing random walk on 5 states. The exercises compute the probability of winning a game for specific values of  $p$  and  $q$ .

After the first game is over, a second game starts with service passing to the other side, until a *set* is completed. This happens when one side wins at least 6 games with a margin of at least 2 games. A set is completed as soon as the score is one of 6:0, 6:1, 6:2, 6:3, 6:4, 7:5, 8:6 and so on. One set follows another until one side wins the match by winning by at least 2 sets. Therefore, a new Markov chain represents the progress of the set. The absorbing probabilities of this higher level chain represent the probability of winning an individual game. In this new Markov chain for the set, after 11 or 12 games again there is an absorbing random walk on 5 states due to the requirement of winning by at least 2 games.

Finally, tennis games have a 3 or 5 set *match* to declare the overall winner by at least 2 sets, making a third-level Markov chain. Women and junior players play 3 set matches and tennis has additional rules for tiebreakers.

### 9.3. Basketball

This section assumes familiarity with the rules and terminology of basketball. The Markov chain model assumes the states and transition probabilities of a basketball game between teams A and B are the following.

**AOff:** Team A goes on offense.

**APen:** Penetrating offense by team A.

**AScore:** Basket scored by team A.

**Bdef:** Ball in possession of team B in defense.

**BOff:** Team B goes on offense.

**BPen:** Penetrating offense by team B.

**BScore:** Basket scored by team B.

**ADef:** Ball in possession of team A in defense.

$p_{\text{eff},A}$ : Probability of organizing a penetrating offense by team A.

$p_{\text{eff},B}$ : Probability of organizing a penetrating offense by team B.

$p_{d,A}$ : Probability of successful defense by team A.

$p_{d,B}$ : Probability of successful defense by team B.

$p_{r,A}$ : Probability of offensive rebound by team A.

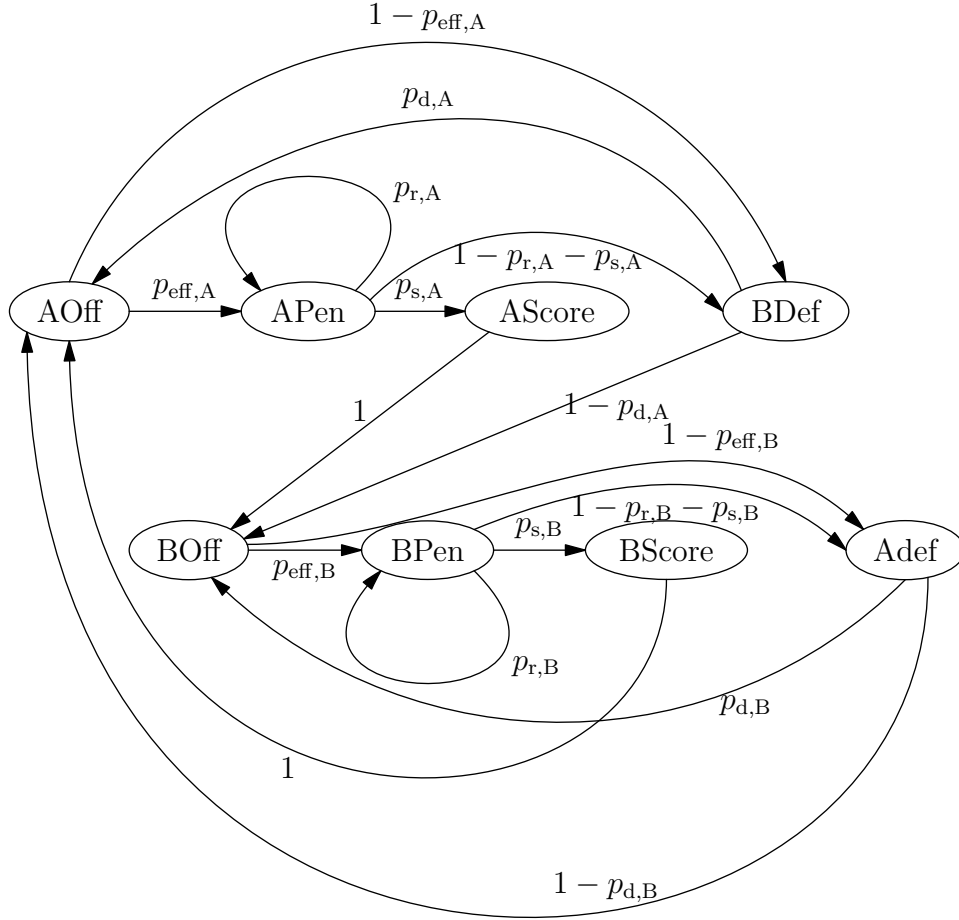
$p_{r,B}$ : Probability of offensive rebound by team B.

$p_{s,A}$ : Probability of scoring a basket by team A as a result of a penetrating offense.

$p_{s,B}$ : Probability of a scoring a basket by team B as a result of a penetrating offense.

A diagram of the states and transition probabilities is in Figure 9.2. This model does not consider three-point shots and scoring by foul shots. This simple Markov chain model could be the basis for extending the model with more states and using advanced sports analytics for the transition probabilities.

College basketball games have 40 minutes playing time for both the men's and women's leagues. The games last longer because of time-outs and foul shots stopping the clock, which this model does not take into account. In a typical game,



**Figure 9.2.** The state transition diagram for a game of basketball.

each team will have about 70 to 80 possessions, measured here as being in the state “AOff” and “BOff”, because starting in this state leads ultimately to either a score “AScore” or a turnover “BDef”.

As an example, take  $p_{\text{eff},A} = 0.6$  and  $p_{\text{eff},B} = 0.75$ , so team A is not as good offensively as team B. It is reasonable to set  $p_{d,A} = 1 - p_{\text{eff},B}$  and  $p_{d,B} = 1 - p_{\text{eff},A}$ . Set  $p_{r,A} = p_{r,B} = 0.3$ . Set  $p_{s,A} = 0.7$  and  $p_{s,B} = 0.6$  so that while team A is not as effective on offense, once it gets near the basket team A scores better than team B near the basket. Then in sample paths with 450 steps in the Markov chain, A has about 75 possessions and an average final score around 89 and B also has about 75 possessions with an average final score around 99. With these parameters, having a more effective offense is more important for winning than better scoring percentage near the basket. Averaging over multiple samples can give a statistical look at the influence of various parameters for winning this simple Markov chain model of basketball. This is an example where sample path properties are more important than stationary probabilities. See the exercises for more details.

## 9.4. Chapter Ending Answer

For tennis, the game points create a reasonable Markov chain model of a game. The probability a player can make a point against as opponent is the analytic measure. The sets and matches can be similarly modeled as Markov chains. For basketball, the teams are in successive states of offense, near the basket, scoring, and turnovers. Sports analytic measures can give the transition probabilities between states.

## 9.5. Chapter Summary

### Key Concepts.

- (1) Tennis can be modeled as a Markov chain with two absorbing states.
- (2) Basketball can be modeled as a Markov chain. The sample path of the chain predicts the final score of the game.

### Vocabulary.

- (1)
- (2)

### Notation.

- (1)

## 9.6. Sources

This section is adapted from [SS93], Sections 3.2, 3.5, 3.9, 3.10, 3.13.

## 9.7. Algorithms and Scripts

**Data:** Transition probability matrix  $P$ , starting state

**Result:** Either absorption probabilities and waiting time to absorption or sample path of the chain

- 1 *Initialization and sample paths*
- 2 Load Markov chain library
- 3 Set state names, set transition probability matrix, set start state
- 4 Determine absorption probabilities and waiting times OR
- 5 Set an example length and create a sample path of example length
- 6 Find sample paths and count scores.

**R:** R script for tennis.

```

1 library("markovchain")
2
3 rows <- 17
4
5 p <- 0.51
6 q <- 1-p
7

```



```

8 P <- matrix(0, rows, rows)
9 P[1, 2] <- q; P[1,3] <- p;
10 P[2, 4] <- q; P[2,5] <- p;
11 P[3, 5] <- q; P[3,6] <- p;
12 P[4, 7] <- q; P[4,8] <- p;
13 P[5, 8] <- q; P[5,9] <- p;
14 P[6, 9] <- q; P[6,10] <- p;
15 P[7, 16] <- q; P[7,11] <- p;
16 P[8, 11] <- q; P[8,14] <- p;
17 P[9, 14] <- q; P[9,12] <- p;
18 P[10,12] <- q; P[10,17] <- p;
19 P[11,16] <- q; P[11,13] <- p;
20 P[12,15] <- q; P[12,17] <- p;
21 P[13,16] <- q; P[13,14] <- p;
22 P[14,13] <- q; P[14,15] <- p;
23 P[15,14] <- q; P[15,17] <- p
24 P[16,16] <- 1;
25 P[17,17] <- 1;
26
27 tennis <- new("markovchain", transitionMatrix=P,
28               name="Tennis")
29
30 print( summary(tennis) )
31
32
33 cat("Probability A wins game: ",
34     absorptionProbabilities(tennis)[1,2], "\n")
35
36 T = P[1:15,1:15]
37 eye = diag(15)
38 N = solve(eye-T, eye)
39 ones = matrix(1, 15,1)
40 VarW = (2*N-eye) %*% N %*% ones - (N %*% ones)^2
41
42 cat("Expected length of game in serves: ",
43     meanAbsorptionTime(tennis)[1],
44     "Standard deviation: ", sqrt(VarW[1]), "\n")

```

R script for basketball.

```

1 library("markovchain")
2
3 rows <- 8
4
5 peffA <- 0.6
6 peffB <- 0.75
7
8 pdA <- 1-peffB
9 pdB <- 1 - peffA

```

```

10
11 prA <- 0.3
12 prB <- 0.3
13
14 psA <- 0.7
15 psB <- 0.6
16
17 stateNames <- c("AOff", "APen", "AScore", "Bdef",
18                 "BOff", "BPen", "BScore", "ADef")
19 P <- matrix(c(0, peffA, 0, 1-peffA, 0, 0,
20               0, 0,
21               0, prA, psA, 1-prA-psA, 0, 0,
22               0, 0,
23               0, 0, 0, 0, 1, 0,
24               0, 0,
25               pdA, 0, 0, 0, 1-pdA, 0,
26               0, 0,
27               0, 0, 0, 0, 0,
28               peffB, 0, 1-peffB,
29               0, 0, 0, 0, 0, prB,
30               psB, 1-prB-psB,
31               1, 0, 0, 0, 0, 0,
32               0, 0,
33               1-pdB, 0, 0, 0, pdB, 0,
34               0, 0),
35             nrow=rows, byrow=TRUE)
36 rownames(P) <- stateNames
37 colnames(P) <- stateNames
38
39 startState <- "AOff"
40
41 bball <- new("markovchain", transitionMatrix=P,
42             states=stateNames, name="Basketball"
43             )
44 print( summary(bball) )
45
46 pathLength <- 450
47 ngames <- 100
48 allAScores <- numeric(ngames)
49 allBScores <- numeric(ngames)
50
51 for (i in 1:ngames) {
52   bballHistory <- rmarkovchain(n=pathLength,
53                               object=bball,
54                               t0=startState)
55   allAScores[i] <- 2 * sum(bballHistory == "AScore"
56 )

```

```
46     allBScores[i] <- 2 * sum(bballHistory == "BScore"  
47   )  
48 }  
49 cat("Mean A Scores: ",      mean(allAScores),  
50     "Standard Deviation: ", sd(allAScores), "\n")  
51 cat("Mean B Scores: ",      mean(allBScores),  
52     "Standard Deviation: ", sd(allBScores), "\n")
```

## 9.8. Problems to Work for Understanding

Chapter 9: Modeling Sports with Markov Chains.

9.1: In tennis, assume A has probability  $p = 0.6$  of winning a point. What is the probability of A winning a game? If  $p = 0.51$ , what is the probability of A winning a game? What is the expected length and the standard deviation of the length of the game in serves for each of these probabilities?

9.2: For the Markov chain model of basketball with the given transition probabilities, what are the expected scores of the two teams?

9.3: Discuss a Markov chain model of ice hockey.

## Modeling Epidemics as a Markov Chain

Markov chain **Susceptible-Infected-Removed (SIR) models** have a population and a disease which infects members of the population for a fixed amount of time, after which the infected individuals are removed, in the sense that each one is no longer susceptible and cannot become infected again. The **Greenwood Model** assumes the number of Infectives in generation  $t$  is a binomial random variable with parameters  $S_t$  and infection success constant  $p$ , not depending on the number of Infectives. The **Reed-Frost model** includes an infective size dependency that the Greenwood model lacks.

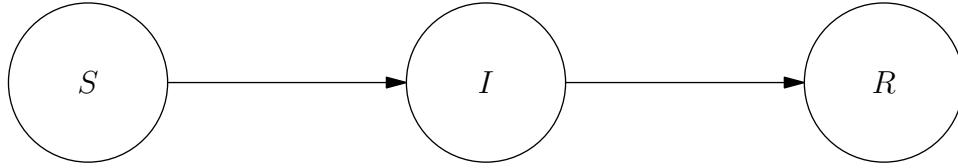
Mathematically Mature: contains mathematics beyond calculus with proofs.

### 10.1. Chapter Starter Question

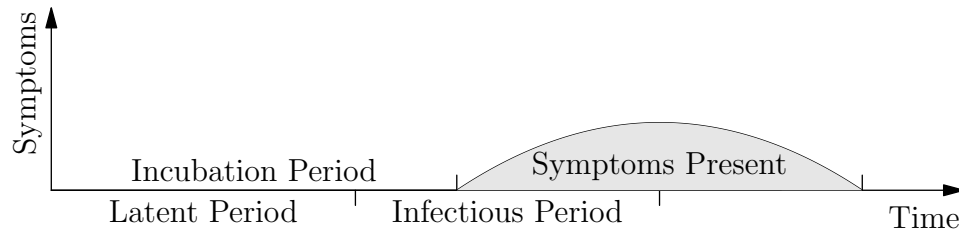
Suppose a single person in a population of  $S$  susceptible individuals has a communicable disease. What is a simple probabilistic model of how this person can infect some number of susceptible individuals in a given time interval?

### 10.2. Introduction

This chapter is an introduction to **Susceptible-Infected-Removed (SIR) models**, using Markov chains. These Markov chains model a population and a disease that infects members of the population for a fixed amount of time, after which each infected individual is removed, in the sense that they are no longer susceptible and cannot become infected again. The removed class includes individuals who are no longer susceptible either because of recovery and subsequent immunity or because of death. That is, after members of the population have been infected for one time unit, the model no longer considers them, as the removed individuals cannot infect anyone else, nor can they become infected again. Therefore only two classes need to



**Figure 10.1.** Schematic class diagram for the simple Susceptible-Infective-Removed epidemic model illustrating the classes of the epidemic and the movement from class to class and not the state transitions of the Markov chain.



**Figure 10.2.** Possible relation of disease stages or periods.

be considered, the Susceptibles and the Infectives. Figure 10.1 shows the movement between the classes.

Markov chain epidemic models use discrete time and a discrete state space. The discrete time will be in units of the infectivity period of the disease. Typically this unit time is about 7-8 days for measles, and about 7-9 days for influenza. Call each of these unit time periods a generation, enumerated by the integer variable  $t$ . (This is a slight change from the usual notation for discrete time Markov chains using the index  $n$  for the discrete time.) The infectivity period may either be distinct from, or overlap, the period when the infected person shows symptoms of the disease. The incubation period, the period between infection and onset of symptoms, and the latent period, the time from infection to infectiousness are different from the infectivity period. Figure 10.2 illustrates one possible configuration of these disease periods. The states will be the number of Susceptibles and Infectives in a homogeneous and well-mixed population. Assume the epidemic takes place over a short enough time interval that the population is a constant value  $N$ , that is, assume no births and no emigration or immigration. It is enough to consider only Susceptibles and Infectives since the number of individuals in the Removed class is determined from the other two.

To keep track of each group, denote the number of Susceptibles at generation  $t$  by  $S_t$ , and the number of Infectives at generation  $t$  by  $I_t$ . These random variables may achieve any integer value such that  $S_t + I_t$  is in the population range.

A natural first question for any epidemic model is the probability of having  $I_{t+1}$  Infectives at generation  $t + 1$ . In asking this question at generation  $t$ , the number of Susceptibles and Infectives at every generation up to  $t$  are known. Since the model is expressed in time units of infectivity periods where individuals move from one class to another, the main focus is on the number of Infectives at generation  $t$ ,

ignoring the past, also keeping track of the Susceptibles. Then the model is a first-order Markov process through the states  $S_t, I_t$  with  $S_t + I_t \leq N$ . If the population is  $N$ , the number of states is  $(N+1)(N+2)/2$  (see the exercises) so this is a Markov chain with many states. Because of the relatively large number of states, this is the first example of a Markov chain without an explicit transition probability matrix, instead giving the transition probability to a new state as a function of the current state.

### 10.3. Greenwood Model

The **Greenwood Model** assumes the number of Infectives in generation  $t$  is a binomial random variable with parameters  $S_t$  and infection success constant  $p$ , not depending on the number of Infectives:

$$\begin{aligned} \mathbb{P}[I_{t+1} = i_{t+1} \mid S_0 = s_0, I_0 = i_0, \dots, S_t = s_t, I_t = i_t] = \\ \mathbb{P}[I_{t+1} = i_{t+1} \mid S_t = s_t, I_t = i_t] = \binom{s_t}{i_{t+1}} p^{i_{t+1}} (1-p)^{s_t - i_{t+1}}. \end{aligned}$$

The first equality represents the first-order Markov chain assumption. Consider the second equality in further detail. At generation  $t$  there are  $s_t$  Susceptibles. To find the probability that  $i_{t+1}$  members of this group become Infectives, choose  $i_{t+1}$  of the Susceptibles who will become infected. Similarly  $p$  is the probability that a given Susceptible will become infected in one generation. Thus the probability  $i_{t+1}$  Susceptibles become Infectives is  $p^{i_{t+1}}$ . Note that a Susceptible becoming Infective is a “success” (for the disease, not the population) in the binomial random variable sense. Remaining a Susceptible is a failure in the binomial sense. The transition for the Susceptibles is

$$S_{t+1} = S_t - I_{t+1}.$$

Because  $I_{t+1}$  is a binomial random variable

$$E[I_{t+1} \mid S_t] = pS_t.$$

This expression gives us the expected number of Infectives at generation  $t+1$  given the number of Susceptibles at generation  $t$ . Extend this idea to say

$$\mathbb{E}[S_{t+1} \mid S_t] = \mathbb{E}[S_t] - \mathbb{E}[I_{t+1}] = (1-p)S_t.$$

By induction

$$\begin{aligned} \mathbb{E}[S_t \mid S_0 = s_0] &= (1-p)^t s_0, \\ \mathbb{E}[I_t \mid S_0 = s_0] &= p(1-p)^{t-1} s_0. \end{aligned}$$

### 10.4. Reed-Frost Model

The Reed-Frost model is an SIR mathematical model of epidemics created in the 1920s by Lowell Reed and Wade Hampton Frost at Johns Hopkins University. Originally presented in a talk by Frost in 1928 and used in courses at Hopkins for two decades, the mathematical formulation was not published until the 1950s.

The Greenwood model has a fixed probability of infection, independent of the number of Infectives at the current generation step. The **Reed-Frost model** includes an infective size dependency that the Greenwood model lacks. The Reed-Frost model is based on the following assumptions:

- (1) The infection is spread directly from Infectives to Susceptibles by a certain type of contact (termed “adequate contact”) and in no other way.
- (2) Any Susceptible in the group, after such contact with an Infective in a given generation, will develop the infection and will be infectious to others only within the following generation period. In subsequent generation periods, the infected individual is wholly and permanently immune and moves to the Removed class.
- (3) Each individual has a fixed probability  $p$  of coming into adequate contact with any other specified individual in the group within one time interval, and this probability is the same for every member of the group.
- (4) The population is constant with no births, immigration or emigration.
- (5) These conditions stay constant during the epidemic.

Set the following initial parameters:

- the size of the population  $N$ ,
- the number of individuals already immune, typically 0,
- the number of Infective cases, usually set at 1,
- the probability  $p$  of adequate contact.

If  $p$  is the probability of a given Susceptible *making adequate contact* with 1 specific Infective, then  $q = 1 - p$  is the probability of *avoiding* adequate contact with that infective. Make the (vastly simplifying and probably unjustified) assumption that all interactions of the Susceptible with all Infectives are independent events. Then  $q^{i_t}$  is the probability the given Susceptible at generation  $t$  avoids adequate contact at generation  $t$  from *all* Infectives in the population at that generation and remains Susceptible at generation  $t + 1$ . This is a failure for the epidemic in the binomial random variable sense. The probability of a Susceptible being infected is then  $(1 - q^{i_t})$ , a success for the epidemic. Then as a binomial random variable, the probability of the number of Infectives in the next generation is

$$\mathbb{P}[I_{t+1} = i_{t+1} \mid S_t = s_t, I_t = i_t] = \binom{s_t}{i_{t+1}} (1 - q^{i_t})^{i_{t+1}} (q^{i_t})^{s_t - i_{t+1}}$$

and  $S_{t+1} = S_t - I_{t+1}$ . In comparison to the Greenwood model, the Reed-Frost model gives a higher probability to more new Infectives at generation  $t + 1$  if the population already has a large number of Infectives at generation  $t$  than if there is only a small population of Infectives. The Reed-Frost model has a positive feedback effect on infectives.

A success for the epidemic is a failure for the Susceptibles and a failure for the epidemic is a success for the Susceptibles. Then an alternative expression for the Susceptibles in the Reed-Frost model is

$$\mathbb{P}[S_{t+1} = s_{t+1} \mid S_t = s_t, I_t = i_t] = \binom{s_t}{s_t - s_{t+1}} (q^{i_t})^{(s_t - s_{t+1})} (1 - q^{i_t})^{s_{t+1}}$$

using  $I_{t+1} = S_t - S_{t+1}$ .

Define the **extinction time**  $\tau$  of an epidemic to be the generation at which  $i_t$  is first zero. This is an absorbing state for the Markov chain. If the number of Susceptibles becomes 0 in a generation  $t$ , then  $i_{t+1} = 0$ . Of more interest is the probability  $S_\tau > 0$  and  $I_\tau = 0$ . Consider an epidemic for which the Infectives have progressed to extinction  $i_1, i_2, \dots, i_{\tau-1}, i_\tau = 0$  with  $i_{\tau-1} > 0$ . Thus

$$\begin{aligned} \mathbb{P}[I_1 = i_1, \dots, I_k = i_k, I_{k+1} = 0 \mid S_0 = n, I_0 = m] = \\ \mathbb{P}[I_1 = i_1 \mid S_0 = n, I_0 = m] \times \mathbb{P}[I_2 = i_2 \mid S_1 = n - i_1, I_1 = i_1] \times \dots \times \\ \mathbb{P}[I_\tau = 0 \mid S_{\tau-1} = s_{\tau-1}, I_{\tau-1} = i_{\tau-1}]. \end{aligned}$$

In this specific epidemic, the **total damage** of the epidemic is  $K = \sum_{j=0}^{\tau} I_j$ . As  $K$  is the sum of  $I_i$ s, treat it as a random variable. Thus consider:

$$\mathbb{P}[K = k \mid S_0 = n, I_0 = m] = \sum_{\vec{i}: |\vec{i}|=k} \mathbb{P}[I_1 = i_1, \dots, I_\tau = 0 \mid S_0 = n, I_0 = m].$$

Some common asymptotics apply here. Let  $m = I_0 = o(N)$  and suppose  $q = e^{-\lambda/N}$  so  $p = 1 - q = O(N^{-1})$  and the expected number of adequate contacts  $q^{i_t}$  is approximately constant at the beginning of the epidemic. Using the first formulation of the Reed-Frost model

$$\mathbb{P}[I_{t+1}] = \text{Bin}(S_t, 1 - e^{-\lambda I_t/N}) \approx \text{Bin}(N, \lambda I_t/N) \approx \text{Poisson}(\lambda I_t).$$

This means  $I_{t+1}$  is the sum of  $I_t$  independent Poisson random variables with parameter  $\lambda$ . That is, the number of Infectives is the result of a Galton-Watson process or branching process. Then from the standard theory for branching processes, the epidemic is *subcritical* if  $\lambda \leq 1$  and *supercritical* if  $\lambda > 1$ . That is, the trajectories of this process either die out or explode in an exponential way, at least at the beginning of the epidemic while the asymptotic assumptions hold. This points to more general stochastic process models of epidemics as branching processes. Although the epidemic models are Markov chains, the tools of branching processes are more applicable and yield more detailed results.

## 10.5. Limitations

Both of these models assume a homogeneous population, i.e. everyone is equally likely to get sick assuming the same exposure. Also the Reed-Frost model assumes that the population mixes perfectly, that is, every Susceptible interacts with every Infective and thus has an equally likely chance to get sick from each one. Both models assume independence in these interactions. These assumptions apply best to a moderately-sized (reasonably) closed situations such as a dormitory, a nursing home under quarantine, a cruise ship, a factory, or perhaps a small town.

For large populations such as a city or an entire country, the assumptions of homogeneous population and perfect mixing don't apply. Also for large populations, direct calculation of the binomial coefficients at each stage is inconvenient, and so using continuum limits is appropriate, leading to differential equation epidemic models. However, one advantage of the stochastic process models is the possibility



of obtaining a distribution for the extinction times. This is a more realistic property than the extinction time given by an asymptotic deterministic model.

More detailed models have multiple health and infection classes instead of just Infectives. More detailed models may also cross these with factors influencing mixing, such as age, social class, or geographical location. The mathematical modeling of epidemics has a huge literature, the references below are a starting point.

## 10.6. Chapter Ending Answer

One particularly simple model is that the infective transmits the disease to a fixed number of susceptibles, this is not probabilistic. A probabilistic model is that the infective transmits to each susceptible with probability  $p$ , leading to the binomial probability distribution of the Greenwood model. A third possibility is that the number of infected is a Poisson random variable with parameter  $\lambda$ . This would be appropriate if the population is large and the transmission rate is constant across various size groups of susceptibles.

## 10.7. Chapter Summary

### Key Concepts.

- (1) Markov chain **Susceptible-Infected-Removed (SIR) models**. have a population and a disease which infects members of the population for a fixed amount of time, after which the infected individuals are removed, in the sense that each one is no longer susceptible and cannot become infected again.
- (2) The **Greenwood Model** assumes the number of Infectives in generation  $t$  is a binomial random variable with parameters  $S_t$  and infection success constant  $p$ , not depending on the number of Infectives.
- (3) For the Greenwood model

$$\mathbb{E}[S_t \mid S_0 = s_0] = (1 - p)^t s_0,$$

$$\mathbb{E}[I_t \mid S_0 = s_0] = p(1 - p)^{t-1} s_0.$$

- (4) The **Reed-Frost model** includes an infective size dependency that the Greenwood model lacks.
- (5) In comparison to the Greenwood model, the Reed-Frost model gives a higher probability to more new Infectives at generation  $t+1$  if there are already a large number of Infectives at generation  $t$  than if there is only a small population of Infectives. The Reed-Frost model has a positive feedback effect on infectives.
- (6) Under some common asymptotic assumptions, is, the number of Infectives is the result of a Galton-Watson process or branching process. Then from the standard theory for branching processes, the epidemic is *subcritical* if  $\lambda \leq 1$  and *supercritical* if  $\lambda > 1$ .

### Vocabulary.

- (1) Markov chain **Susceptible-Infected-Removed (SIR) models**. have a population and a disease which infects members of the population for a fixed

amount of time, after which the infected individuals are removed, in the sense that each one is no longer susceptible and cannot become infected again.

- (2) The **Greenwood Model** assumes the number of Infectives in generation  $t$  is a binomial random variable with parameters  $S_t$  and infection success constant  $p$ , not depending on the number of Infectives.
- (3) The **Reed-Frost model** includes an infective size dependency that the Greenwood model lacks.
- (4) The **extinction time  $\tau$  of an epidemic** to be the generation at which  $i_t$  is first zero.
- (5) The **total damage** of the epidemic is  $K = \sum_{j=0}^{\tau} i_j$ .

#### Notation.

- (1)  $t$  – the integer variable enumerating unit time periods for each generation
- (2)  $N$  – population constant value
- (3)  $S_t$  – the number of Susceptibles at generation  $t$
- (4)  $I_t$  – the number of Infectives at generation  $t$
- (5)  $p$  – the probability that a given Susceptible will become infected in one generation
- (6)  $K = \sum_{j=0}^{\tau} I_j$  – the total damage of the epidemic
- (7)  $q = 1 - p$  – the probability of *avoiding* contact with that infective
- (8)  $\tau$  – extinction time of an epidemic to be the generation at which  $i_t$  is first zero
- (9)  $s_t$  – random number of Susceptibles at time  $t$
- (10)  $i_t$  – random number of Infectives at time  $t$
- (11)  $m = I_0 = o(N)$
- (12)  $\lambda$  – parameter such that  $q = e^{-\lambda/N}$

### 10.8. Sources

Details of the Greenwood and Reed-Frost models are from “Criticality in Epidemic Models” by R. Dolgoarshinnykh [Dol]. Comments on epidemics as branching processes and more detailed assumptions for epidemics are from “Branching Processes: Their Role in Epidemiology”, by C. Jacob [Jac10]. See also [SR13] for a survey of mathematical models of infectious diseases. The spatial epidemic exercise is adapted from the Ohio Supercomputer Center Summer Institute, Reed-Frost Epidemic Model.

### 10.9. Reading Suggestion:

### 10.10. Outside Readings and Links:

- (1) *Introduction to Probability*, Grinstead and Snell. Chapter 11 - Markov Chains - <http://tinyurl.com/qw6sa>
- (2) Generalized Markov Models of Infectious Disease Spread

## (3) Criticality in Epidemic Models

## 10.11. Algorithms and Scripts

**Data:** initial Susceptibles, Infectives, probability, time**Result:** Plot of Susceptibles, Infectives versus time1 *Initialization*

2 Set initial Susceptibles, Infectives, probability, time

3 Loop over time

4 Get random binomial variate from number of Susceptible

5 Update the infectives

6 **return** *Plot of Susceptibles, Infectives versus time***Algorithm 12:** Simulation of epidemics with Greenwood and Reed Frost models.**R:** R script for Greenwood model.

```

1 S0 <- 999
2 I0 <- 1
3 p <- 0.2
4
5 T <- 30
6 S <- numeric(T + 1)
7 I <- numeric(T + 1)
8
9 S[1] <- S0
10 I[1] <- I0
11 for (t in 2:(T + 1)) {
12     I[t] <- rbinom(1, size=S[t-1], prob=p)
13     S[t] <- S[t - 1] - I[t]
14 }
15
16 plot(1:(T + 1), S, col="blue",
17      xlim = c(0, (T + 1)), ylim=c(0, (S0 + I0)),
18      main="Greenwood Epidemic Model",
19      xlab="Time", ylab="S, I")
20 points(1:(T + 1), y=I, col="red")

```

R script for Reed-Frost model.

```

1 S0 <- 9999
2 I0 <- 1
3 p <- 0.00001
4 q <- 1 - p
5
6 T <- 25
7 S <- numeric(T + 1)
8 I <- numeric(T + 1)

```

```

9
10 S[1] <- S0
11 I[1] <- I0
12 for (t in 2:(T + 1)) {
13     QT = q^I[t-1]
14     I[t] <- rbinom(1, size=S[t-1], prob=1-QT)
15     S[t] <- S[t - 1] - I[t]
16 }
17
18 plot(1:(T + 1), S, col="blue",
19      xlim = c(0, (T + 1)), ylim=c(0, (S0 + I0)),
20      main="Reed-Frost Epidemic Model",
21      xlab="Time", ylab="S, I")
22 points(1:(T + 1), y=I, col="red")

```

## 10.12. Problems to Work for Understanding

Chapter 10: Markov Chain Epidemic Models.

10.1: If the population is  $N$  and  $S_t + I_t \leq N$ , explain why the number of states is  $(N + 1)(N + 2)/2$ .

10.2: Write a script that simulates a place-based epidemic model. For this model, assume the individuals stand at the vertices of a two-dimensional square grid. Let one individual be an infective case. An infective can now probabilistically infect only his immediate neighbors on the grid. In the next time period, those people who got sick now have a chance to infect their neighbors and so on. Display on a two-dimensional grid that shows all the individuals what state they are in (i.e., Susceptible, Infective, or Recovered), with an animation if possible. Run the script many times with different input parameters. How does the pattern of the epidemic flow change with the contact probability?



## Reversible Markov Chains

Assume  $X$  is an irreducible and positive recurrent chain, started at its unique stationary distribution  $\pi$ . This means  $X_0$  has distribution  $\pi$ , and all successive  $X_n$  have distribution  $\pi$  as well. Now suppose that, for every  $n$ , the sequence of random variables  $X_1, X_2, \dots, X_n$  has the same joint distribution as the time-reversed sequence  $X_n, X_{n-1}, \dots, X_1$ . Then the chain  $X$  is **reversible** and its stationary distribution  $\pi$  is also said to be reversible. This means a video record of a long sample path of a reversible chain started from the stationary distribution looks the same if the video is run backwards. The goal of this chapter is to characterize reversible Markov chains and their properties.

Mathematically Mature: contains mathematics beyond calculus with proofs.

### 11.1. Chapter Starter Question

Imagine a video is made of the Ehrenfest urn model started in its stationary distribution. Would it be possible to distinguish whether the video is played forward or in reverse simply by viewing the video and observing the movement of the balls between the urns?

### 11.2. Detailed Balance Equations

If the sequence of random variables  $X_1, X_2, \dots, X_n$  from a Markov chain has the same joint distribution as the time-reversed sequence  $X_n, X_{n-1}, \dots, X_1$ , then the chain  $X$  is **reversible**. The script in this chapter illustrates this property with the weather in Oz example. Reversing a long sample path from the weather Markov chain, then using the Maximum Likelihood Estimator

$$\hat{p}_{ij}^{\text{MLE}} = \frac{n_{ij}}{\sum_{\nu} n_{i\nu}}$$

where  $n_{ij}$  is the number of transitions from  $X_n = i$  to  $X_{n+1} = j$  gives approximately the original transition probability matrix. This indicates, within the limits of the

simulation and estimation, that the reversed chain has the same joint distribution as the original weather chain. In fact, the transition probability matrix estimated from a reversed sample path being approximately the same as the original transition probability matrix indicates that the weather in Oz Markov chain is reversible. See [Spe17] for more details.

**Proposition 11.1.** *If an irreducible and positive recurrent Markov chain is started from the stationary distribution  $\pi$ , then the time-reversed chain has the Markov property.*

**Proof.** Since the Markov chain is irreducible and positive recurrent, there is a stationary distribution  $\pi$ . Since the Markov chain is started in the stationary distribution  $\pi$ , the distribution of the state at step  $\ell$  is  $\pi$ . Then

$$\begin{aligned} & \mathbb{P}[X_\ell = i \mid X_{\ell+1} = j, X_{\ell+2} = i_{\ell+2}, \dots, X_n = i_n] \\ &= \frac{\mathbb{P}[X_\ell = i, X_{\ell+1} = j, X_{\ell+2} = i_{\ell+2}, \dots, X_n = i_n]}{\mathbb{P}[X_{\ell+1} = j, X_{\ell+2} = i_{\ell+2}, \dots, X_n = i_n]} \\ &= \frac{\pi_i P_{ij} P_{ji_{\ell+2}} \cdots P_{i_{n-1}i_n}}{\pi_j P_{ji_{\ell+2}} \cdots P_{i_{n-1}i_n}} \\ &= \frac{\pi_i P_{ij}}{\pi_j} \end{aligned}$$

which depends only on  $i$  and  $j$ , so the time-reversed chain has the Markov property.  $\square$

**Remark 11.2.** The definition of reversibility is inconvenient because it does not give an effective way to check if the chain is time-reversible. The following theorem gives an easy criterion and can even help find the stationary distribution  $\pi$ , see Theorem 11.7.

**Theorem 11.3** (Reversibility Condition). *An irreducible and positive recurrent Markov chain is reversible if and only if the state space has a probability distribution  $\pi$  such that*

$$\pi_i P_{ij} = \pi_j P_{ji}$$

*for all  $i$  and  $j$  and then  $\pi$  is the unique stationary distribution.*

**Remark 11.4.** The condition

$$\pi_i P_{ij} = \pi_j P_{ji}$$

is the **detailed balance equation**. This condition says that starting from the stationary distribution

$$\mathbb{P}[X_n = i, X_{n+1} = j] = \mathbb{P}[X_n = j, X_{n+1} = i]$$

so the chain transitions from  $i$  to  $j$  as often as it transitions from  $j$  to  $i$ . This accounts for term “balance” in “detailed balance equation”.

**Proof. ( $\Rightarrow$ ):** From the proof of the Proposition, the time-reversed sequence of random variables satisfies

$$\mathbb{P}[X_\ell = i \mid X_{\ell+1} = j] = \frac{\pi_i P_{ij}}{\pi_j}.$$

If the Markov chain is reversible, the previous expression must be the same as the forward transition probability  $\mathbb{P}[X_{\ell+1} = i \mid X_\ell = j] = P_{ji}$ . Then the detailed balance equation holds.

( $\Leftarrow$ ): From the proposition, the time-reversed chain is Markov. If the original and the time-reversed chain both start at the same stationary distribution and satisfy the detailed balance equations, then the transition probabilities between arbitrary states  $i$  and  $j$  are the same from  $i$  to  $j$  or back from  $j$  to  $i$ . Then the random variables  $X_1, X_2, \dots, X_n$  has the same joint distribution as the time-reversed sequence  $X_n, X_{n-1}, \dots, X_1$ . By definition the chain is reversible.  $\square$

**Example 11.5.** If the  $k \times k$  transition probability matrix is symmetric, then  $\pi = (1/k, \dots, 1/k)$  satisfies the detailed balance equation and the corresponding Markov chain is reversible.  $\nabla$

**Remark 11.6.** If there exist 2 states such that  $P_{ij} > 0$  but  $P_{ji} = 0$  then the detailed balance equation fails, since the limiting probabilities of all entries of an irreducible and positive recurrent chain are nonzero. Then the chain is not reversible.

**Theorem 11.7.** Assume the Markov chain is irreducible and positive recurrent and probability distribution  $\pi$  satisfies the detailed balance equations

$$\pi_i P_{ij} = \pi_j P_{ji}.$$

- (1) The distribution  $\pi$  is the stationary distribution of the chain.
- (2) The chain is reversible.

**Proof.** Using the detailed balance equations

$$\sum_j \pi_j P_{ji} = \sum_j \pi_i P_{ij} = \pi_i \sum_j P_{ij} = \pi_i.$$

Since the chains is irreducible and positive recurrent, then  $\pi$  must be the unique stationary distribution.  $\square$

### 11.3. Kolmogorov's Loop Criterion

A transition probability matrix is *reversible* if the corresponding Markov chain is reversible.

**Definition 11.8.** The equality condition

$$(11.1) \quad P_{j_0 j_1} P_{j_1 j_2} \cdots P_{j_{\ell-1} j_\ell} P_{j_\ell j_0} = P_{j_0 j_\ell} P_{j_\ell j_{\ell-1}} \cdots P_{j_2 j_1} P_{j_1 j_0}$$

is called **Kolmogorov's loop criterion**.  $\diamond$

**Theorem 11.9** (Kolmogorov loop criterion). An irreducible and positive recurrent Markov chain is reversible if and only if

$$P_{j_0 j_1} P_{j_1 j_2} \cdots P_{j_{\ell-1} j_\ell} P_{j_\ell j_0} = P_{j_0 j_\ell} P_{j_\ell j_{\ell-1}} \cdots P_{j_2 j_1} P_{j_1 j_0}$$

for every finite sequence of distinct states  $j_0, j_1, \dots, j_\ell$ .



**Proof. ( $\Rightarrow$ ):** An irreducible and positive recurrent Markov chain has a nonzero stationary distribution  $\pi$ . Since the Markov chain is reversible, the detailed balance equations hold, so  $P_{ij} = \frac{\pi_j P_{ji}}{\pi_i}$  for every  $i$  and  $j$ . Substituting this relation for every probability on the left side of the loop criterion

$$P_{j_0 j_1} P_{j_1 j_2} \cdots P_{j_{\ell-1} j_\ell} P_{j_\ell j_0} = \frac{\pi_{j_1} P_{j_1 j_0}}{\pi_{j_0}} \cdot \frac{\pi_{j_2} P_{j_2 j_1}}{\pi_{j_1}} \cdots \frac{\pi_{j_\ell} P_{j_\ell j_{\ell-1}}}{\pi_{j_{\ell-1}}} \cdot \frac{\pi_{j_0} P_{j_0 j_\ell}}{\pi_{j_\ell}}.$$

Canceling the  $\pi_i$  factors and reversing the order of multiplication gives the right side of the Kolmogorov loop criterion.

( $\Leftarrow$ ): Assume the loop criterion holds. Fix states  $j_\ell$  and  $j_0$ . Then

$$\begin{aligned} \mathbb{P}[X_\ell = j_\ell, X_{\ell-1} = j_{\ell-1}, \dots, X_2 = j_2, X_1 = j_1 \mid X_0 = j_0] = \\ P_{j_0 j_1} P_{j_1 j_2} \cdots P_{j_{\ell-1} j_\ell} P_{j_\ell j_0} = \frac{P_{j_0 j_\ell}}{P_{j_\ell j_0}} P_{j_\ell j_{\ell-1}} \cdots P_{j_3 j_2} P_{j_2 j_1} P_{j_1 j_0} = \\ \frac{P_{j_0 j_\ell}}{P_{j_\ell j_0}} \mathbb{P}[X_\ell = j_0, X_{\ell-1} = j_1, \dots, X_2 = j_{\ell-2}, X_1 = j_{\ell-1} \mid X_0 = j_\ell] \end{aligned}$$

where the second equality is a rearrangement of the  $\ell$ -step loop criterion. Now sum both sides over all choices of the intermediate states  $j_1, j_2, \dots, j_{\ell-1}$  to obtain the following relation among the  $n$  step transition probabilities

$$P_{j_0 j_\ell}^n = \frac{P_{j_0 j_\ell}}{P_{j_\ell j_0}} P_{j_\ell j_0}^n.$$

Multiply by  $P_{j_\ell j_0}$  and take the limit in  $n$  on both sides and use that the limits of the multi-step transition probabilities are the stationary probabilities, guaranteed to exist since the Markov chain is irreducible and positive recurrent. The result is

$$\pi_{j_0} P_{j_0 j_\ell} = \pi_{j_\ell} P_{j_\ell j_0}$$

which is exactly the reversibility criterion. □

**Remark 11.10.** In words, Kolmogorov's loop criterion says a Markov transition matrix is reversible if and only for every loop of distinct states, the forward loop probability product equals the backward loop probability product.

**Remark 11.11.** If the transition matrix is symmetric, then  $P_{ij} = P_{ji}$  for all  $i, j$ , so Kolmogorov's loop criterion is always satisfied and the chain is reversible.

For a two-state Markov chain Kolmogorov's loop criterion is always satisfied since  $P_{12}P_{21} = P_{12}P_{21}$ .

Usually loop checking involves much computational work. The obvious reason is that the number of loops that need to be checked grows very quickly with  $n$  where  $n$  is the number of states. The number of loops can be expressed as the number of cycles in the complete graph on  $n$  nodes. See Table 11.1. The following Proposition counts the number of equations that must be checked to apply Kolmogorov's loop criterion.

$k$	1	2	3	4	5	6	7	8	9	10
equations	0	0	1	7	37	197	1,172	8,018	62,814	556,014

**Table 11.1.** Number of equation to be checked for a Markov chain with  $k$  states.

**Proposition 11.12.** *For an  $k$  state Markov chain, with  $k \geq 3$ , the number of equations that must be checked for reversibility by Kolmogorov's method is*

$$\sum_{\nu=3}^n \binom{n}{\nu} \frac{(\nu-1)!}{2}.$$

**Proof.** (1) For a 3-state Markov chain, only 1 equation

$$P_{12}P_{23}P_{31} = P_{13}P_{32}P_{21}$$

needs checking, since all 2 step loops automatically satisfy the criterion and any other length 3 loop over the same states results in the same equation after rearranging the multiplication order.

- (2) For  $n = 4$ , all 2 step loops automatically satisfy the criterion. Next check each loop of 3 states. For 3 state loops, choose any 3 of 4 states and there is one equation for each. Finally, for each loop of 4 states, fix the starting state. Then the other 3 states have  $3!$  possible orders. However, the other side of the equation is just the reversed path, so there are only  $\frac{3!}{2}$  paths involving 4 states with the first state fixed. In total, the number of loop equations is

$$\binom{4}{3} + \binom{4}{4} \frac{3!}{2}$$

which can be written as

$$\binom{4}{3} \frac{(3-1)!}{2} + \binom{4}{4} \frac{(4-1)!}{2}$$

which corresponds to the conclusion of the proposition.

- (3) The previous argument easily generalizes to larger values of  $n$ .

□

## 11.4. An Algorithm for Determining Reversibility

Next define operations to transform transition matrices in such a way as to preserve their reversibility status (either reversible or non-reversible). These transformations will be useful in creating new reversible Markov chains from existing ones, and for checking reversibility of Markov chains. A *row multiplication operation* on row  $i$  of a Markov transition matrix is the multiplication of row  $i$  by a positive constant leaving the sum of the non-diagonal elements at most 1, followed by an adjustment to  $p_{ii}$  to make the row sum exactly 1. A *column multiplication operation* on column  $j$  of a Markov transition matrix is the multiplication of column  $j$  by a positive constant of allowable size (so no row sums exceed 1) followed by adjustments to all diagonal entries to make every row sum exactly 1.

**Lemma 11.13.** *A Markov chain matrix  $P$  maintains its reversibility status after a row multiplication operation or a column multiplication operation.*

- Proof.** (1) The Kolmogorov loop criterion states that  $P$  is reversible if and only if for all loops of distinct states, the forward loop probability product equals the backward loop probability product.
- (2) Let the  $i$ th row of  $P$  correspond to state  $i$ . If a loop does not include state  $i$ , then a multiplication row operation on row  $i$  has no effect on the forward and backward loop products.
- (3) Otherwise, state  $i$  appears in the first subscript of a forward loop probability if and only if it appears in the first subscript in the corresponding adjacent transition probability in the backward loop probability. See equation (11.1).
- (4) So the row operation will have an identical effect on both sides of the loop product. Equality is maintained.
- (5) A similar conclusion holds for column product operations.

□

**Remark 11.14.** Let  $P^{(*)}$  be the matrix resulting from a row (or column) multiplication operation on  $P$ , then the limiting probabilities for  $P^{(*)}$  in the lemma are generally different from the limiting probabilities for  $P$ .

If the matrix  $P$  is an  $k \times k$  transition probability matrix, then at most  $k - 1$  row or column multiplication operations will determine if  $P$  is reversible.

**Data:** Transition probability matrix  $P$

**Result:** Symmetric matrix  $P^{(*)}$

```

1 Pick two symmetric positions in  $P$  with non-zero entries, say  $P_{i_1 i_2}$  and
   $P_{i_2 i_1}$ .
2  $S \leftarrow \{i_1, i_2\}$ .
3  $j \leftarrow i_1, \ell \leftarrow i_2$ 
4 repeat
5   if  $P_{j\ell} = P_{\ell j}$  then
6     | Move to the next step.
7   else if  $P_{j\ell} < P_{\ell j}$  then
8     | Multiply row  $\ell$  by  $P_{j\ell}/P_{\ell j}$ 
9     | Adjust  $P_{\ell\ell}$  to make the  $\ell$  row sum 1.
10  else if  $P_{j\ell} > P_{\ell j}$  then
11    | Multiply column  $\ell$  by  $P_{\ell j}/P_{j\ell}$ 
12    | Adjust the diagonal elements to make the row sums 1.
    // The new matrix  $P^{(*)}$  will now have  $P_{j\ell}^{(*)} = P_{\ell j}^{(*)}$ .
    Choose another state  $i_3 \notin S$  which has nonzero transition probabilities
    to a state in  $S$ .
13   $j \leftarrow i_3, \ell \notin S$  with  $P_{\ell i_3} \neq 0$ 
14   $S \leftarrow \{i_1, i_2, i_3\}$ .
15 until There are no more states left to add
    // After  $k-1$  steps  $S = \{1, \dots, k\}$ .
    Let  $P^{(*)}$  be the final matrix.

```

**Algorithm 13:** Algorithm for determining reversibility

**Theorem 11.15.** *Let  $P$  be a  $k \times k$  transition matrix to which the Algorithm is applied, resulting in  $P^{(*)}$ . Then  $P$  is reversible if and only if  $P^{(*)}$  is symmetric.*

**Proof.** (1) ( $\Rightarrow$ )

- (a) Assume  $P$  is reversible, then by the lemma,  $P^{(*)}$  is reversible.
- (b) Let  $\phi = (\phi_1, \dots, \phi_k)$  be the stationary distribution for  $P^{(*)}$ .
- (c) Note that  $P^{(*)}$  is formed so that  $P_{ij}^{(*)} = P_{ji}^{(*)}$  for a particular subcollection of  $(i, j)$  pairs which will include each of  $1, 2, \dots, k$  somewhere among the subcollection of transitions  $(i, j)$ .
- (d) Let  $(i, j)$  be one of the transition pairs in the collection. Since  $P^{(*)}$  is reversible, the detailed balance equations  $\phi_i P_{ij}^{(*)} = \phi_j P_{ji}^{(*)}$  must hold for the pair  $(i, j)$ .
- (e) Using the equality from the symmetry,  $\phi_i = \phi_j$ .
- (f) But all the states  $1, \dots, k$  appear in the set of transitions somewhere in the collection, so  $\phi_1 = \phi_2 = \dots = \phi_k$ .
- (g) Now take an arbitrary pair  $(i, j)$ . Since  $P^{(*)}$  is reversible, the detailed balance holds for all  $i, j$ . Hence  $\phi_i P_{ij}^{(*)} = \phi_j P_{ji}^{(*)}$  for all  $i, j$ .
- (h) Since  $\phi_i = \phi_j$ , for all pairs  $(i, j)$  then  $P_{ij}^{(*)} = P_{ji}^{(*)}$ , so  $P^{(*)}$  is symmetric.

(2) ( $\Leftarrow$ )

If  $P^{(*)}$  is symmetric, then  $P^{(*)}$  is reversible, so by the lemma  $P$  is reversible.

□

**Remark 11.16.** The Algorithm chooses the smaller of 2 matrix entries to change the matrix  $P$ . Also corrections are made to the diagonal elements in order to ensure the rows sum to 1. In fact, by examining the loop equation (11.1), correction of the diagonal elements is not necessary and the transformed matrix  $P^{(*)}$  no longer needs to be a transition matrix. The proof shows the important issue is whether  $P^{(*)}$  is symmetric or not.

**Example 11.17.** Let

$$P = \begin{pmatrix} 17/40 & 0 & 3/40 & 1/2 \\ 0 & 11/20 & 1/4 & 1/5 \\ 3/10 & 1/4 & 9/20 & 0 \\ 1/2 & 1/20 & 0 & 9/20 \end{pmatrix}.$$

To check for reversibility, transform  $P$  by column or row operations. First, the zeroes of  $P$  are symmetric, and  $P_{14} = P_{41}$ , so symmetry for states  $\{1, 4\}$  already exists. Now make the  $(1, 3)$  entry match the  $(3, 1)$  entry without losing the  $(1, 4)$  and  $(4, 1)$  symmetry. It is possible to multiply column 3 by  $(3/10)/(3/40) = 4$  or row 3 by  $(3/40)/(3/10) = 1/4$ . Make the latter choice to obtain a new matrix with row 3 equal to  $(3/40, 1/16, 9/80, 0)$ . This is not a transition probability matrix because the row no longer sums to 1, so change the diagonal element at  $(3, 3)$  to  $1 - 3/40 - 1/16 = 69/80$ . Now the transformed matrix is

$$P^{(1)} = \begin{pmatrix} 17/40 & 0 & 3/40 & 1/2 \\ 0 & 11/20 & 1/4 & 1/5 \\ 3/40 & 1/16 & 69/80 & 0 \\ 1/2 & 1/20 & 0 & 9/20 \end{pmatrix}.$$

Now the set of included states is  $S = \{1, 4, 3\}$ , so state 2 needs to be included. To preserve the values in  $(1, 4)$  and  $(4, 1)$ , and  $(1, 3)$  and  $(3, 1)$ , only row 2 or column 2 can be changed. Choose to multiply column 2 by 4 to make entries  $(4, 2)$  and  $(2, 4)$  equal. The result is

$$P^{(2)} = \begin{pmatrix} 17/40 & 0 & 3/40 & 1/2 \\ 0 & 11/5 & 1/4 & 1/5 \\ 3/40 & 1/4 & 69/80 & 0 \\ 1/2 & 1/5 & 0 & 9/20 \end{pmatrix}.$$

Adjust the entries in the diagonal positions in rows 2, 3, 4 to make the matrix a transition probability matrix

$$P^{(*)} = \begin{pmatrix} 17/40 & 0 & 3/40 & 1/2 \\ 0 & 11/20 & 1/4 & 1/5 \\ 3/40 & 1/4 & 27/40 & 0 \\ 1/2 & 1/5 & 0 & 3/10 \end{pmatrix}.$$

Now  $P$  is reversible if and only if  $P^{(*)}$  is reversible. But  $P^{(*)}$  is symmetric so it is automatically reversible. Using the detailed balance equations makes it easy to compute the stationary distribution of  $P$ , see the exercises.

▽

### 11.5. Examples of Reversible Chains

**The Weather in Oz.** For the familiar example of the weather in Oz, the transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} \end{matrix}.$$

Using the stationary distribution  $(\frac{2}{5}, \frac{1}{5}, \frac{2}{5})$ , the detailed balance equations show that the Markov chain is reversible. See the exercises.

The single equation to check for the Kolmogorov loop criterion is

$$P_{RN}P_{NS}P_{SR} = P_{RS}P_{SN}P_{NR},$$

that is,

$$\frac{1}{4} \cdot \frac{1}{2} \cdot \frac{1}{4} = \frac{1}{4} \cdot \frac{1}{4} \cdot \frac{1}{2}$$

which is true, so the Markov chain is reversible.

The state  $N$  communicates with the other two states, so the criterion in the exercises also shows this Markov chain is reversible.

**Negative Drift Random Walk on the Non-negative Integers.** Consider a negative drift simple random walk, restricted to be non-negative by a reflecting boundary. That is,  $P_{01} = 1$  and otherwise  $P_{i,i+1} = p < 0.5$ ,  $P_{i,i-1} = 1 - p > 0.5$  for  $i > 0$ . The detailed balance equations are

$$\begin{aligned} \pi_0 &= (1 - p)\pi_1 \\ p\pi_i &= (1 - p)\pi_{i+1} \end{aligned}$$

so  $\pi_1 = \pi_0/(1 - p)$ ,  $\pi_2 = p\pi_0/(1 - p)^2$  and in general  $\pi_n = p^{n-1}\pi_0/(1 - p)^n$ . Since  $\sum_{\nu} \pi_{\nu} = 1$ ,

$$\pi_0 \left( 1 + \frac{1}{1 - p} \sum_{\nu=0}^{\infty} \left( \frac{p}{1 - p} \right)^{\nu} \right) = 1.$$

Because  $\frac{p}{1-p} < 1$  the geometric series converges and

$$\begin{aligned} \pi_0 &= \frac{1}{2} \cdot \frac{1 - 2p}{1 - p} \\ \pi_n &= \left( \frac{1}{2} - p \right) \left( \frac{p^{n-1}}{(1 - p)^{n+1}} \right)^n, n \geq 1. \end{aligned}$$

With these values, by Theorem 11.7,  $\pi$  is the stationary distribution and the Markov chain is reversible.

**Random Walks on Weighted Graphs.** A *random walk on a weighted graph* is a general and common example of a reversible Markov chain. Assume the undirected edge between vertices  $i$  and  $j$  in a connected graph has a weight  $w_{ij} = w_{ji}$ . The Markov chain is irreducible because the graph with edge weights greater than 0 is connected. When at  $i$ , the walker goes to  $j$  with probability proportional to  $w_{ij}$ , so

$$P_{ij} = \frac{w_{ij}}{\sum_{\nu} w_{i\nu}}.$$

Let

$$s = \sum_{i,j} w_{ij}$$

be the sum of all weights and let

$$\pi_i = \frac{\sum_{\nu} w_{i\nu}}{s}.$$

The transition probability matrix is reversible because

$$\pi_i P_{ij} = \frac{\sum_{\nu} w_{i\nu}}{s} \cdot \frac{w_{ij}}{\sum_{\nu} w_{i\nu}} = \frac{w_{ij}}{s} = \frac{w_{ji}}{s} = \frac{\sum_{\nu} w_{j\nu}}{s} \cdot \frac{w_{ji}}{\sum_{\nu} w_{j\nu}} = \pi_j P_{ji}.$$

It is not necessary to forbid self-edges, some edges  $w_{ii}$  may be nonzero. However,  $w_{ii}$  appears only once in the sum  $s$ , while the value  $w_{ij}$  appears twice, once each for  $i$  and  $j$ .

In the simple case with no self-edges and all nonzero weights equal to 1, the stationary distribution is

$$\pi_i = \frac{\text{degree}(i)}{2 \cdot (\text{number of edges})}.$$

**Ehrenfest Urn Model.** The physicist P. Ehrenfest proposed the following model for statistical mechanics and kinetic theory. The motivation is diffusion through a membrane. Two urns labeled  $A$  and  $B$  contain a total of  $N$  balls. In the Ehrenfest urn model a ball is selected at random with all selections equally likely, and moved from the urn it is in to the other urn. The state at each time is the number of balls in the urn  $A$ , from 0 to  $N$ . Then the transition probability matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ \frac{1}{N} & 0 & 1 - \frac{1}{N} & 0 & \cdots & 0 & 0 \\ 0 & \frac{2}{N} & 0 & 1 - \frac{2}{N} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \frac{1}{N} \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}.$$

The balls fluctuate between the two containers with a drift from the one with the larger number of balls to the one with the smaller number.

A stationary distribution for this Markov chain has entry  $\pi_i = \binom{N}{i}/2^N$ . This is the binomial distribution on  $N$ , so that for large  $N$ , the normal distribution approximates the distribution of balls. This conclusion is plausible given the physical origin of the Markov chain as a model for diffusion. All states are accessible and all states communicate so the chain has a stationary distribution. The chain is periodic with period 2 so it is not regular.

To show the Markov chain is reversible requires

$$\begin{aligned}\pi_0 P_{01} &= \pi_1 P_{10}, \\ \pi_i P_{i,i+1} &= \pi_{i+1} P_{i+1,i}, \\ \pi_N P_{N,N-1} &= \pi_{N-1} P_{N-1,N}.\end{aligned}$$

See the exercises.

### 11.6. Chapter Ending Answer

It should not be possible to distinguish whether the video is played forward or in reverse simply by viewing the video and observing the movement of the balls between the urns. The distribution of the balls is stationary, or in physical terms, in equilibrium. That is, a ball is as likely to move from urn A to urn B in forward time, or from urn B to urn A in reverse time. Observing the movement of balls between the urns provides no clue about the time direction of the video.

### 11.7. Chapter Summary

#### Key Concepts.

- (1) A Markov chain with stationary distribution  $\pi$  is reversible if and only if the state space has a probability distribution  $\pi$  such that

$$\pi_i P_{ij} = \pi_j P_{ji}$$

for all  $i$  and  $j$  and  $\pi$  is the unique stationary distribution.

- (2) The condition says that starting from the stationary distribution

$$\mathbb{P}[X_n = i, X_{n+1} = j] = \mathbb{P}[X_n = j, X_{n+1} = i]$$

so the chain transitions from  $i$  to  $j$  as often as it transitions from  $j$  to  $i$ .

- (3) Assume the Markov chain is irreducible and positive recurrent and probability distribution  $\pi$  satisfies the detailed balance equation

$$\pi_i P_{ij} = \pi_j P_{ji}.$$

Then the distribution  $\pi$  is the stationary distribution of the chain and the chain is reversible.

- (4) Let  $P$  be a  $k \times k$  transition matrix to which an Algorithm of row and column operations is applied, resulting in  $P^{(*)}$ . Then  $P$  is reversible if and only if  $P^{(*)}$  is symmetric.

#### Vocabulary.

- (1) Assume  $X$  is an irreducible and positive recurrent chain, started at its unique stationary distribution  $\pi$ . This means  $X_0$  has distribution  $\pi$ , and all other  $X_n$  have distribution  $\pi$  as well. Now suppose that for every  $n$ , the sequence of random variables  $X_1, X_2, \dots, X_n$  has the same joint distribution as the time-reversed sequence  $X_n, X_{n-1}, \dots, X_1$ , then the chain  $X$  is **reversible**.



- (2) The condition

$$\pi_i P_{ij} = \pi_j P_{ji}$$

is the **detailed balance equation**.

- (3) **Kolmogorov's loop criterion** is

$$P_{j_0 j_1} P_{j_1 j_2} \cdots P_{j_{k-1} j_k} P_{j_k j_0} = P_{j_0 j_k} P_{j_k j_{k-1}} \cdots P_{j_2 j_1} P_{j_1 j_0}$$

for every finite sequence of distinct states  $j_0, j_1, \dots, j_k$ .

#### Notation.

- (1)  $X, X_0, X_n$  – Markov chain, starting state, general step of the chain.
- (2)  $k$  – Number of states in the Markov chain.
- (3)  $\pi, \pi_i$  – Stationary distribution and general element of the stationary distribution.
- (4)  $i, j, i_\ell$  etc. – arbitrary states of the Markov chain.
- (5)  $P, P_{ij}$  – Transition probability matrix and general element of transition probability matrix.
- (6)  $P^{(*)}$  – the matrix resulting from a row (or column) multiplication operation on  $P$ .

### 11.8. Sources

The definition of reversibility, the Proposition, and the Reversibility Condition Theorem are adapted from Gravner.

Remarks surrounding the Reversibility Condition Theorem are adapted from Chen and Sigman.

Identifying reversibility with the Kolmogorov loop condition is adapted from Brill et al. [BhCHJ18]. The proof that the Kolmogorov Loop Criterion is equivalent to reversibility is adapted from Kolmogorov's Criterion

The example of the negative drift random walk on the non-negative integers is adapted from Sigman.

The example of the random walk on a connected graph is adapted from Gravner.

The problem about the random walk of a king on a checkerboard is inspired by a problem in Gravner.

### 11.9. Reading Suggestion:

#### 11.10. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)

### 11.11. Algorithms and Scripts

**Data:** Transition probability matrix

**Result:** Maximum Likelihood Estimator of reversed chain

1 *Initialization of Matrices*

2 Initialize state names and transition probability matrix  $P$ ; Create new Markov chain object; Run Markov chain for a long time and record sample path; Reverse the sample path; Create Maximum Likelihood Estimator of transition probability matrix;

**Algorithm 14:** Illustration of Reversible Markov Chains.

**R:** R script for reversiblechain.R.

```

1
2 library("markovchain")
3
4 weatherStates <- c("Rain", "Nice", "Snow")
5 byRow <- TRUE
6 weatherMatrix <- matrix(
7   data=c(1/2, 1/4, 1/4, 1/2, 0, 1/2, 1/4, 1/4, 1/2),
8   byrow = byRow, nrow = 3,
9   dimnames = list(weatherStates, weatherStates))
10 mcWeather <- new("markovchain",
11   states = weatherStates, byrow = byRow,
12   transitionMatrix = weatherMatrix, name="Weather")
13 weatherDays <- rmarkovchain(n = 2000, object =
14   mcWeather, t0 = "Nice")
15 reverseWeather <- rev(weatherDays)
16
17 weatherFittedMLE <- markovchainFit(data =
18   reverseWeather, method = "mle")
19 weatherFittedMLE$estimate

```

### 11.12. Problems to Work for Understanding

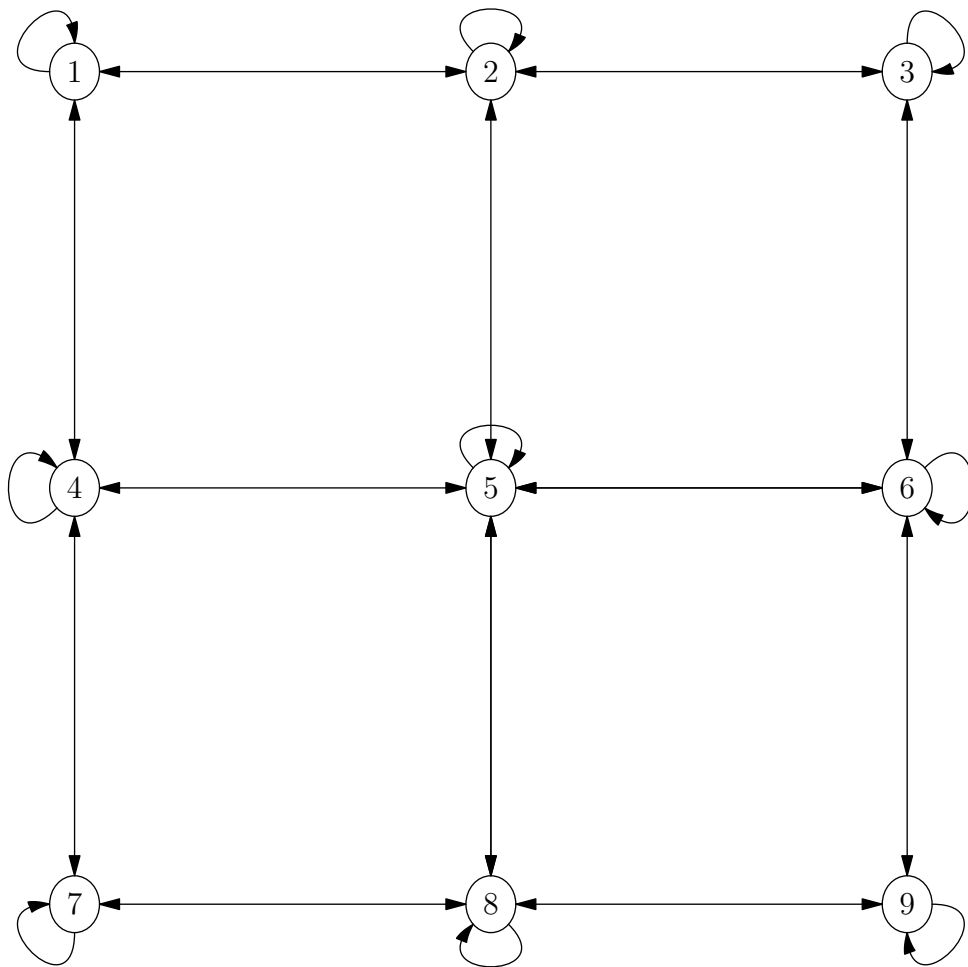
Chapter 11: Reversible Markov Chains.

11.1: Use the detailed balance equations to show the weather in Oz Markov chain is reversible.

11.2: Compute the stationary distribution for

$$P = \begin{pmatrix} 17/40 & 0 & 3/40 & 1/2 \\ 0 & 11/20 & 1/4 & 1/5 \\ 3/10 & 1/4 & 9/20 & 0 \\ 1/2 & 1/20 & 0 & 9/20 \end{pmatrix}$$

using the detailed balance equations.



**Figure 11.1.** A  $3 \times 3$  square lattice graph with uniform transition probabilities.

11.3: Consider the  $3 \times 3$  square lattice graph in Figure 11.1. The graph has 9 vertices with 12 edges between nearest lattice neighbors and self-loops at each vertex. If a vertex has  $n$  neighbors then the probability of moving to a neighboring vertex or staying at the vertex is  $\frac{1}{n+1}$  uniformly. Find the stationary distribution for the random walk on this graph.

11.4: In the game of Checkers, a “king” can move from a black square to any adjacent black square on an  $8 \times 8$  square array colored alternately red and black.

- (a) Assuming the king starts at one of the two corner squares of the chessboard, compute the expected number of steps before it returns to the starting position.
- (b) Now assume two kings start at opposite corner squares, and move independently (and may occupy the same square). What is now the expected

number of steps before they simultaneously occupy their starting positions again?

11.5: Complete the proof that the number of loops to check in Kolmogorov's loop criterion is

$$\sum_{\nu=3}^n \binom{n}{\nu} \frac{(\nu-1)!}{2}$$

for general  $n$ .

11.6: Show that if a Markov chain has a state accessible to and from every other state in exactly 1 step (i.e. the  $j_0$  row and  $j_0$  column of the transition matrix have nonzero entries), then for the Kolmogorov loop criterion it is sufficient to check loops of only three states. (However, it is possible that no such state exists.)



## Lumped Markov Chains

Partitioning the states of a Markov chain into equivalence classes or lumps and viewing the dynamics at a coarser level as the system of interest moves among the lumps is often convenient. Examples of such aggregation include a weather model lumping the states “rain” and “snow” into one state called “bad weather” or a physical model aggregating the microstates of a physical system into coarse grained “mesostates” representing many microstates. Other examples are reducing the size of the PageRank matrix used in web searches, and modeling clusters or “communities” in networks.

Although the dynamics moving among the lumps is not necessarily Markovian in general, there is a natural requirement for a Markov chain model on the set of lumped states. This requirement matches the time evolution of the original unlumped chain started at equilibrium. This provides bounds on the error of the dynamics predicted by the lumped chain considered as a model of the unlumped chain. The goal in this chapter is to analyze the accuracy of such coarse grained models compared to the exact microscopic behavior, i.e. to bound the error in a coarse grained description.

Mathematically Mature: contains mathematics beyond calculus with proofs.

### 12.1. Chapter Starter Question

The weather in the land of Oz, where it is either rainy, nice or snowy, has transition probability matrix

$$P = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} \end{matrix}.$$

Consider lumping the weather states into only “good” days with nice weather and “bad” days with rainy or snowy weather. What is the probability of going from a bad weather day to a bad weather day?

## 12.2. Lumpable Markov Chains

**Definition 12.1.** Let  $X_n$  be a Markov chain with state space  $\mathcal{X} = \{x_1, x_2, \dots, x_k\}$  and initial distribution  $X_0$ . Given a partition  $\hat{\mathcal{S}} = \{E_1, E_2, \dots, E_v\}$  of the state space  $\mathcal{X}$  into  $v$  equivalence classes, define a new stochastic process  $\hat{X}_n$  as follows: At the  $j$ th step, the state of the new chain is the set  $E_\xi$  when  $E_\xi$  contains the state of the  $j$ th step of the original chain. Think of the notation  $\hat{X}_n$  as “heaping up” the chain into the lumps. Assign the transition probabilities for  $\hat{X}_n$  as follows: The initial distribution is

$$\mathbb{P}[\hat{X}_0 = E_\xi] = \mathbb{P}_{X_0}[x_0 \in E_\xi].$$

Given the initial state, the transition probability for the first step is

$$\mathbb{P}[\hat{X}_1 = E_\eta \mid \hat{X}_0 = E_\xi] = \mathbb{P}_{X_0}[X_1 \in E_\eta].$$

In general for the  $n$ th step

$$\begin{aligned} \mathbb{P}[\hat{X}_{n+1} = E_\eta \mid \hat{X}_n = E_{\eta_n}, \hat{X}_{n-1} = E_{\eta_{n-1}}, \dots, \hat{X}_1 = E_{\eta_1}, \hat{X}_0 = E_\xi] \\ = \mathbb{P}_{X_0}[x_{n+1} \in E_\eta \mid x_n \in E_{\eta_n}, x_{n-1} \in E_{\eta_{n-1}}, \dots, x_1 \in E_{\eta_1}, x_0 \in E_\xi]. \end{aligned}$$

Call this new process  $\hat{X}_n$  a lumped process and if the lumped process is a Markov chain, it is a **lumped chain** of the Markov chain  $X_n$ . Sometimes this is also called a *projection* of the Markov chain  $X_n$ .  $\diamond$

Figure 12.1 has a schematic diagram of a lumped Markov chain. A lumped process of a given Markov chain need not be a Markov chain in general, see the second example below.

**Definition 12.2.** A Markov chain  $X_n$  on the state space  $\mathcal{X}$  is said to be **lumpable** with respect to a partition  $\hat{\mathcal{S}}$  of  $\mathcal{X}$  if for every starting distribution  $X_0$  the lumped chain  $\hat{X}_n$  is a Markov chain with state space  $\hat{\mathcal{S}}$  and the associated transition probabilities do not depend on the choice of  $X_0$ .  $\diamond$

The following theorem gives a necessary and sufficient condition for a Markov chain to be lumpable.

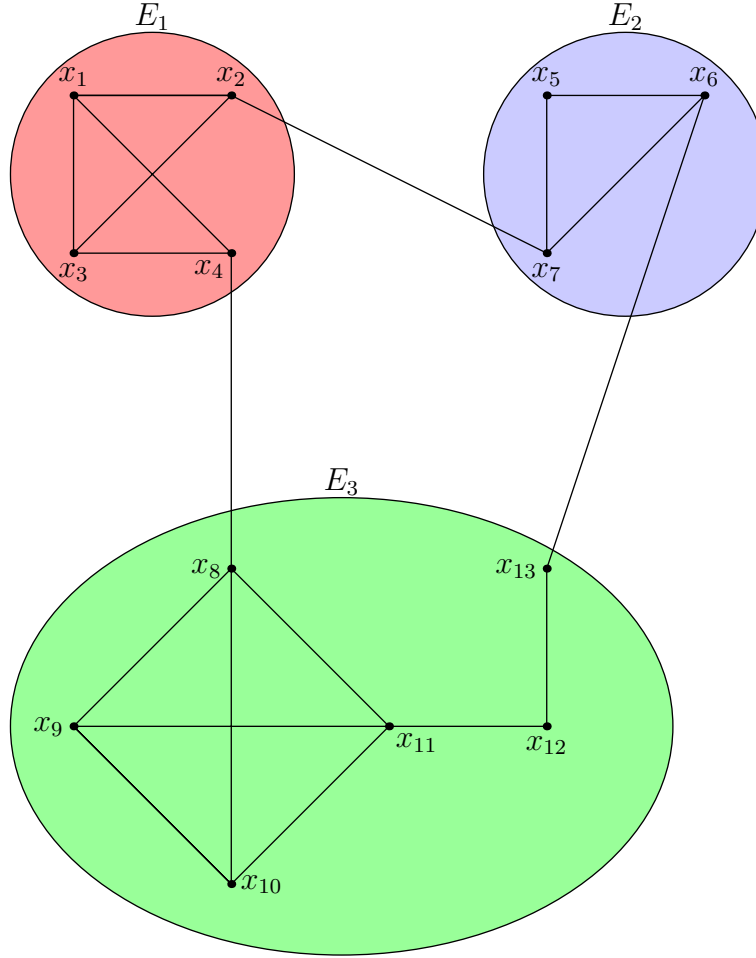
**Theorem 12.3.** Denote the transition probability of the Markov chain  $X_n$  from state  $x_i$  to state  $x_j$ , for  $i, j = 1, \dots, k$ , by  $P_{ij}$ . The Markov chain  $X_n$  is lumpable with respect to the partition  $\hat{\mathcal{S}}$  if and only if for every pair of sets  $E_\xi$  and  $E_\eta$ ,  $\sum_{x_\nu \in E_\eta} P_{i\nu}$  has the same value for every  $x_i \in E_\xi$ . These common values form the transition probabilities  $\hat{P}_{\xi\eta}$  for the lumped chain.

**Proof.** ( $\Rightarrow$ ) (a) If the chain is lumpable, then

$$\mathbb{P}[\hat{X}_1 = E_\eta \mid \hat{X}_0 = E_\xi] = \mathbb{P}_{X_0}[X_1 \in E_\eta]$$

is the same for every  $X_0$  for which it is defined. Call this common value  $\hat{P}_{\xi,\eta}$ .

- (b) In particular this must be true for  $X_0^{(\nu)}$  having a 1 in its  $\nu$ th component for state  $x_\nu \in E_\xi$ . Hence  $\mathbb{P}_{X_0^{(\nu)}}[x_j \in E_\eta] = \sum_{x_\nu \in E_\eta} P_{i\nu}$  has the same value  $\hat{P}_{\xi\eta}$  for every  $x_i \in E_\xi$ .



**Figure 12.1.** A schematic diagram of a lumped Markov chain.

- ( $\Leftarrow$ ) (a) The proof must show that if the lumpability condition is satisfied, the probability

$$\mathbb{P} \left[ \hat{X}_{n+1} = E_{\eta+1} \mid \hat{X}_n = E_{\eta_n}, \hat{X}_{n-1} = E_{\eta_{n-1}}, \dots, x_1 \in E_{\eta_1}, \hat{X}_0 = E_{\xi} \right]$$

depends only on  $E_{\eta_{n+1}}$  and  $E_{\eta_n}$ .

- (b) By definition, the probability in question is

$$\mathbb{P}_{X_0} [x_{n+1} \in E_{\eta_{n+1}} \mid x_n \in E_{\eta_n}, x_{n-1} \in E_{\eta_{n-1}}, \dots, x_1 \in E_{\eta_1}].$$

- (c) By the Markov memory-less property, this conditional probability may be written in the form  $\mathbb{P}_{\xi'} [x_{n+1} \in E_{\eta_{n+1}}]$  where  $\xi'$  is a probability vector with nonzero components only in the states of  $E_{\eta_n}$ .
- (d) This probability depends on the states in  $E_{\eta_{n+1}}$  and on the states in  $E_{\eta_n}$ .



- (e) By the hypothesis of the lumpability condition,  $\mathbb{P}_{\xi'} [x_{n+1} \in E_{\eta_{n+1}}]$  where  $\xi'$  is a probability vector with nonzero components only in the states of  $E_{\eta_n}$  is  $\hat{P}_{\eta_n \eta_{n+1}}$ , independent of state  $x_n \in E_{\eta_n}$ .
- (f) Thus the probability depends only on  $E_{\eta_{n+1}}$  and  $E_{\eta_n}$ .

□

**Example 12.4.** Recall the example of the weather in the land of Oz, where it is rainy, nice or snowy, with transition probability matrix

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

Now consider lumping the weather states into only “good” days with nice weather and “bad” days with rainy or snowy weather. That is, choose the partition  $\hat{\mathcal{S}} = \{\{N\}, \{R, S\}\} = \{G, B\}$ . The probabilities of moving from  $R$  to  $N$  and from  $S$  to  $N$  are the same. The complementary probabilities of moving from  $R$  or  $S$  to  $\{R, S\}$  are each the same. The probability of moving from  $N$  to  $\{R, S\}$  or  $\{N\}$  is trivially the same for all states in  $G$ . This weather Markov chain satisfies the lumpability condition. The lumped transition probability matrix is

$$P = \begin{array}{c} \begin{array}{cc} & G & B \\ \begin{array}{c} G \\ B \end{array} & \begin{pmatrix} 0 & 1 \\ 1/4 & 3/4 \end{pmatrix} \end{array}.$$

By direct computation the stationary distribution on the lumped chain is  $(1/5, 4/5)$ , as expected from lumping the stationary distribution of the original weather chain.

On the other hand, the lumpability condition is not satisfied for the partition  $\{\{R\}, \{N, S\}\}$  since  $P_{N\{N, S\}} = 1/2$  but  $P_{S\{N, S\}} = 3/4$ . ▽

**Example 12.5.** An arbitrary lumping of states of a Markov chain does not necessarily lead to a Markov chain. Let  $X_n$  be a Markov chain with state space  $\mathcal{X} = \{1, 2, 3\}$  with  $X_0 = 2$  (or as a probability distribution,  $X_0 = (0, 1, 0)$ ) and transition probability matrix

$$P = \begin{pmatrix} 0.8 & 0.1 & 0.1 \\ 0.2 & 0.7 & 0.1 \\ 0 & 0.1 & 0.9 \end{pmatrix}.$$

Then lump the states as  $E_1 = \{1\}$  and  $E_2 = \{2, 3\}$ . First,

$$\mathbb{P}[\hat{X}_1 = E_2 \mid \hat{X}_0] = \mathbb{P}_{X_0}[X_1 = 2, 3] = 0.7 + 0.1 = 0.8$$

and

$$\begin{aligned} \mathbb{P}[\hat{X}_2 = E_2, \hat{X}_1 = E_2 \mid \hat{X}_0] &= \\ \mathbb{P}_{X_0}[X_2 \geq 2, X_1 = 2] &+ \mathbb{P}_{X_0}[X_2 \geq 2, X_1 = 3] = \\ (0.7 + 0.1) \cdot 0.7 &+ (0.9 + 0.1) \cdot 0.1 = 0.66. \end{aligned}$$

Second,

$$\mathbb{P}[\hat{X}_2 = E_2, \hat{X}_1 = E_1] = \mathbb{P}_{X_0}[X_2 \geq 2, X_1 = 1] = 0.2 \cdot (0.1 + 0.1) = 0.04.$$

Combining probabilities for these two paths

$$\mathbb{P}[\hat{X}_2 = E_2] = \mathbb{P}[\hat{X}_2 = E_2, \hat{X}_1 = E_2] + \mathbb{P}[\hat{X}_2 = E_2, \hat{X}_1 = E_1] = 0.7.$$

Next consider the three step paths

$$\begin{aligned} \mathbb{P}[\hat{X}_3 = E_2, \hat{X}_2 = E_2, \hat{X}_1 = E_1] &= \\ \mathbb{P}_{X_0}[X_1 = 1, X_2 = 2, X_3 \geq 2] &+ \mathbb{P}[X_1 = 1, X_2 = 3, X_3 \geq 2] = \\ 0.2 \cdot 0.1 \cdot (0.7 + 0.1) &+ 0.2 \cdot 0.1 \cdot (0.1 + 0.9) = 0.036. \end{aligned}$$

and

$$\begin{aligned} \mathbb{P}[\hat{X}_3 = E_2, \hat{X}_2 = E_2, \hat{X}_1 = E_2] &= \\ \mathbb{P}_{X_0}[X_3 \geq 2, X_2 = 2, X_1 = 2] &+ \mathbb{P}_{X_0}[X_3 \geq 2, X_2 = 3, X_1 = 2] + \\ \mathbb{P}_{X_0}[X_3 \geq 2, X_2 = 2, X_1 = 3] &+ \mathbb{P}_{X_0}[X_3 \geq 2, X_2 = 3, X_1 = 3] = \\ 0.7 \cdot 0.7 \cdot (0.7 + 0.1) &+ 0.7 \cdot 0.1 \cdot (0.1 + 0.9) + \\ 0.1 \cdot 0.1 \cdot (0.7 + 0.1) &+ 0.1 \cdot 0.9 \cdot (0.1 + 0.9) = 0.56. \end{aligned}$$

Combining the previous two probabilities

$$\mathbb{P}[\hat{X}_3 = E_2, \hat{X}_2 = E_2] = 0.56 + 0.036 = 0.596$$

so

$$\mathbb{P}[\hat{X}_3 = E_2 \mid \hat{X}_2 = E_2] = 0.596/0.7 \approx 0.8514$$

but

$$\mathbb{P}[\hat{X}_3 = E_2 \mid \hat{X}_2 = 2, \hat{X}_1 = E_2] = 0.56/0.66 \approx 0.8485$$

showing that  $\hat{X}_k$  is not a Markov chain.  $\nabla$

A matrix formulation of this theorem for irreducible and aperiodic chains is useful. Define a partition  $\hat{\mathcal{S}} = \{E_1, E_2, \dots, E_v\}$  of the finite state space  $\mathcal{X} = \{x_1, x_2, \dots, x_k\}$  of the underlying Markov chain  $X_n$  which is assumed to be irreducible and aperiodic. Then the Markov chain has a unique stationary distribution  $\boldsymbol{\pi}$ . The **distributing matrix**  $U$  is the wide  $v \times k$  matrix with entries

$$U_{ij} = \begin{cases} \boldsymbol{\pi}_j / \sum_{x_\nu \in E_i} \boldsymbol{\pi}_\nu & x_j \in E_i \\ 0 & \text{otherwise.} \end{cases}$$

The  $i$ th row of the distributing matrix is the stationary distribution restricted to  $E_i$  and renormalized so its entries add to 1.

Let the **collecting matrix**  $V$  be the tall  $k \times v$  matrix where the  $j$ th column,  $j = 1, 2, \dots, v$ , is a vector with 1 in the components corresponding to states in  $E_j$ , and 0 elsewhere. For any probability distribution  $p$  on  $\mathcal{X}$  the collecting matrix specifies the lumped probability distribution  $\hat{p} = pV$  on the partition  $\hat{\mathcal{S}}$ . Then  $UV = I_v$  since  $V$  simply collects back exactly what  $U$  distributes. The lumped transition matrix is  $\hat{P} = UPV$ .

For any probability distribution  $q$  in the lumped space, the image  $qU$  is locally equilibrated, i.e.  $qU$  restricted to any element  $E_j$  of the partition equals the stationary distribution restricted to  $E_j$  and renormalized to add to  $q_j$ . In particular, with  $\hat{\pi} = \pi V$

$$U_{ij} = V_{ji} \frac{\pi_j}{\hat{\pi}_i}, \quad i = 1, \dots, k, j = 1, \dots, v$$

whose  $i$ th row,  $i = 1, 2, \dots, v$ , is the probability vector having equal values for states in  $E_i$  and 0 elsewhere. See the exercises.

Note that the rows of  $PV$  corresponding to the elements in the same set of the partition are the same. See the following example with the weather Markov chain. This will be true in general for a chain satisfying the condition for lumpability. The matrix  $U$  simply removes this duplication of rows. Again, see the following example with the weather Markov chain. The choice of  $U$  is not unique, all that is needed is that the  $i$ th row should be a probability vector with nonzero components only for states in  $E_i$ . (See the exercises for an example with an absorbing chain without a stationary distribution  $\pi$ .) Sometimes for simplicity and convenience, choose the vector with equal components.

Next consider the local equilibration operator  $VU$ . The name is justified by considering its action. Starting from any distribution  $p$  on  $\mathcal{X}$ ,  $VU$  collects the probability in each  $E_j$ , then redistributes this much probability  $pV$  among the lumped states in the partition member  $E_j$  as  $(pU)_j \hat{\pi}_i$ . In particular,

$$\pi = \pi VU.$$

**Example 12.6.** For the land of Oz weather example with

$$\begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix},$$

recall the stationary distribution is  $\pi = (2/5, 1/5, 2/5)$ . With the partition  $\hat{\mathcal{S}} = \{\{N\}, \{R, S\}\} = \{G, B\}$  the distributing matrix is

$$U = \begin{pmatrix} 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix}.$$

For the distribution  $q = (2/3, 1/3)$  on the lumped space,  $qU = (1/6, 2/3, 1/6)$ , so that the  $1/3$  probability of being in the bad weather state is distributed proportionally according to the stationary distribution over the  $R$  and  $S$  states. This explains why  $U$  is called the distributing matrix.

The collecting matrix is

$$V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

For the probability distribution  $p = (1/6, 1/12, 3/4)$  on  $\{R, N, S\}$ , the lumped probability distribution  $\{G, B\}$  is  $\hat{p} = pV = (1/12, 11/12)$ . In particular,

$$\left(\frac{1}{5}, \frac{4}{5}\right) = \hat{\pi} = \pi V = \left(\frac{2}{5}, \frac{1}{5}, \frac{2}{5}\right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The equality  $UV = I_2$  is easy to check.

The lumped weather transition probability matrix is

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

For the probability distribution  $q = (5/6, 1/6)$  on the lumped weather, the image  $qU = (1/12, 5/6, 1/12)$ . Restricting  $qU$  to element  $B$  of the partition gives  $(1/12, 1/12)$ , the uniform distribution  $(2/5, 2/5)$  of the stationary distribution on  $B$  renormalized to total  $1/6$ .

As an example of

$$U_{ij} = V_{ji} \frac{\pi_j}{\pi_i}, \quad i = 1, \dots, v, j = 1, \dots, k$$

consider  $U_{21} = 1/2$  while  $V_{12} \frac{\pi_1}{\pi_2} = 1 \cdot \frac{2/5}{4/5} = 1/2$ .

The rows of

$$PV = \begin{pmatrix} 1/4 & 3/4 \\ 0 & 1 \\ 1/4 & 3/4 \end{pmatrix}$$

corresponding to the  $R$  and  $S$  states in  $B$  are the same. Then multiplying by  $U$  removes the duplication and illustrates why the rows of  $U$  only need to be a probability vector with nonzero components only for states in  $G$  or  $B$ .  $\nabla$

It is convenient to assume that the states in  $\mathcal{X}$  are ordered so that those in  $E_1$  come first, those in  $E_2$  come next and so on with those in  $E_v$  last. From here on, assume that this ordering of states has been made.

**Theorem 12.7.** *If  $P$  is the transition probability matrix of the Markov chain  $X_n$ , then  $X_n$  is lumpable with respect to the partition  $\hat{\mathcal{S}}$  if and only if  $VUPV = PV$ .*

**Proof.** (1)  $(\Rightarrow)$

(a) The matrix  $VU$  has the block matrix form

$$VU = \begin{pmatrix} W_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & W_v \end{pmatrix}$$

where  $W_1, W_2, \dots, W_v$  are probability matrices.

- (b) Since the chain is lumpable, the probability of moving from a state of  $E_i$  to the set  $E_j$  is the same for all states of  $E_i$ , hence the components of a column of  $PV$  corresponding to  $E_j$  are all the same.
- (c) Say that common value of probability is  $\rho_j$ , so a column of  $PV$  is  $\rho_j$  in the entries corresponding to  $E_j$  and 0 elsewhere.
- (d) Then multiplying by  $VU$ , with block probability matrix form, gives a column which is  $\rho_j$  in the entries corresponding to  $E_j$  and 0 elsewhere.
- (e) Therefore the columns form a fixed vector for  $W_j$ , this proves  $VUPV = PV$ .

(2)  $(\Leftarrow)$

- (a) Assume  $VUPV = PV$ . Then the columns of  $PV$  are fixed vectors for  $VU$ .

- (b) But each block  $W_j$  is the transition probability matrix, so its only fixed column vectors are of the form  $c\mathbf{1}$ .
- (c) Hence all the components of a column of  $PV$  corresponding to a set  $E_i$  must be the same, so the chain is lumpable.

□

**Example 12.8.** For the weather example with the ordering of states as  $N, R, S$  to correspond to  $\{G, B\} = \{\{N\}, \{R, S\}\}$ ,

$$VU = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix}.$$

Also

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

and it is quick to check that  $VUPV = PV$ .

▽

**Corollary 12.9.**

$$\hat{P}^n = UP^nV.$$

**Proof.**

$$\hat{P}^2 = (UPV)(UPV) = UP(VUPV) = UP^2V$$

by using the theorem at the last equality. The corollary follows by induction. □

### 12.3. Lumping Positive Recurrent and Aperiodic Chains

Assume the irreducible and aperiodic chain  $X$  with limiting matrix  $\pi$  is lumpable for some partition  $\hat{\mathcal{S}}$ . (Note the abuse of notation where the stationary distribution is identified with the limiting matrix whose rows are the stationary distribution.) The resulting lumped chain will be also be irreducible and aperiodic. Let  $\hat{\pi}$  be the limiting matrix for the lumped chain. Then

$$\begin{aligned} \hat{\pi} &= \lim_{\nu \rightarrow \infty} \frac{\hat{P} + \hat{P}^2 + \cdots + \hat{P}^\nu}{\nu} \\ &= \lim_{\nu \rightarrow \infty} \frac{UPV + UP^2V + \cdots + UP^\nu V}{\nu} \\ &= U \left( \lim_{\nu \rightarrow \infty} \frac{P + P^2 + \cdots + P^\nu}{\nu} \right) V \\ &= U\pi V. \end{aligned}$$

This states that the components of  $\hat{\pi}$  are obtained from  $\pi$  by simply adding the components of the corresponding partition set. From the infinite series representation for the fundamental matrix  $\hat{N}$

$$\hat{N} = UNV.$$

### 12.4. Lumping Absorbing Chains

Assume  $P$  is an absorbing chain. Restrict attention to the case of lumping only states of the same kind. That is, any element of the partition will contain only absorbing states or only nonabsorbing states. Recall that the standard form for an absorbing chain is

$$P = \begin{pmatrix} I & 0 \\ R & Q \end{pmatrix}$$

and write  $U$  in the form

$$U = \begin{pmatrix} U_A & 0 \\ 0 & U_T \end{pmatrix}$$

where entries of  $U_A$  refer to absorbing states and entries of  $U_T$  to transient states. Similarly write  $V$  in the form

$$V = \begin{pmatrix} V_A & 0 \\ 0 & V_T \end{pmatrix}.$$

In terms of this decomposition, the matrix condition for lumpability becomes

$$\begin{aligned} V_A U_A V_A &= V_A \\ V_T U_T R V_A &= R V_A \\ V_T U_T Q V_T &= Q V_T. \end{aligned}$$

Since  $U_A V_A = I$ , the first condition is automatically satisfied. The standard form for the transition matrix  $\hat{P}$  is

$$\hat{P} = U P V = \begin{pmatrix} U_A & 0 \\ 0 & U_T \end{pmatrix} \begin{pmatrix} I & 0 \\ R & Q \end{pmatrix} \begin{pmatrix} V_A & 0 \\ 0 & V_T \end{pmatrix} = \begin{pmatrix} I & 0 \\ U_T R V_A & U_T Q V_T \end{pmatrix}.$$

Then

$$\begin{aligned} \hat{R} &= U_T R V_A \\ \hat{Q} &= U_T Q V_T. \end{aligned}$$

From  $V_T U_T Q V_T = Q V_T$ , obtain  $\hat{Q}^2 = U_T Q V_T U_T Q V_T = U_T Q^2 V_T$  and so on inductively.

From the infinite series representation for the fundamental matrix  $N$

$$\begin{aligned} \hat{N} &= I + \hat{Q} + \hat{Q}^2 + \cdots \\ &= U_T I V_T + U_T Q V_T + U_T Q^2 V_T + \cdots \\ &= U_T (I + Q + Q^2 + \cdots) V_T \\ &= U_T N V_T. \end{aligned}$$

From this  $\hat{\mathbf{w}} = \hat{N} \mathbf{1} = U_T N V_T \mathbf{1} = U_T N \mathbf{1} = U_T \mathbf{w}$  and

$$\begin{aligned} \hat{B} &= \hat{N} \hat{R} = U_T N V_T U_T R V_A \\ &= U_T N R V_A \\ &= U_T B V_A. \end{aligned}$$

So the important absorption quantities are all easily obtained for the lumped chain from the original chain.

A consequence of  $\hat{\mathbf{w}} = U_T \mathbf{w}$  is the following. Let  $E_j$  be any transient set, and let  $x_i$  be a state in  $E_j$ . Choose the  $i$ th row of  $U_T$  to be a probability vector with 1 in the  $x_i$  component. This means for all  $x_\ell$  in  $E_j$ ,  $\mathbf{w}_\ell = \mathbf{w}_i$ . When a chain is lumpable, the mean time to absorption is the same for all starting states in the equivalence set  $E_j$ .

The covariance matrix of the number of visits to a transient state of the lumped process follows easily from the covariance matrix of the original process. The elements of the covariance matrix  $\text{Cov}[Y_{E_i E_j}, Y_{E_i E_l}]$  for the lumped process are

$$\text{Cov}[Y_{E_i E_j}, Y_{E_i E_l}] = \sum_{x_\mu \in E_j, x_\nu \in E_l} \text{Cov}[Y_{i\mu}, Y_{i\nu}]$$

### 12.5. Lumping Reversible Chains

**Theorem 12.10.** *A reversible, irreducible, and aperiodic Markov chain is reversible when lumped.*

**Proof.** Let  $D_\pi$  be the diagonal matrix with the stationary distribution entries along the diagonal. The condition for reversibility can then be written as  $P = D_\pi P^T D_\pi^{-1}$ . Using  $\hat{P} = UPV$  reversibility implies  $\hat{P} = UD_\pi P^T D_\pi^{-1}V$ . The relation  $U_{ij} = V_{ji} \frac{\pi_j}{\pi_i}$  can be written as  $V^T D_\pi^{-1} = D_\pi U$ . Hence  $D_\pi V^T = UD_\pi$  so  $D_\pi V^T = UD_\pi$  and  $D_\pi^{-1}V = U^T D_\pi^{-1}$ . Therefore,

$$\hat{P} = D_\pi V^T P^T U^T D_\pi^{-1}$$

and

$$\hat{P} = D_\pi \hat{P}^T D_\pi^{-1}$$

and the lumped process is reversible.  $\square$

### 12.6. Larger Examples

**Example 12.11.** Consider a random walk of a particle moving along a straight line in unit steps. Each step is 1 unit to the right with probability  $\frac{1}{2}$  and to the left with probability  $\frac{1}{2}$ . The particle moves until it reaches one of two extreme points which are absorbing boundaries. In particular, consider the small case where the state space has 5 values with absorbing boundary states  $x_1$  and  $x_5$  and using the ordering for the standard form the probability transition matrix is

$$P = \begin{matrix} & \begin{matrix} s_1 & s_5 & s_2 & s_3 & s_4 \end{matrix} \\ \begin{matrix} s_1 \\ s_5 \\ s_2 \\ s_3 \\ s_4 \end{matrix} & \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 & 1/2 & 0 \end{pmatrix} \end{matrix}.$$

Take the partition  $S = \{\{s_1, s_5\}, \{s_2, s_4\}, \{s_3\}\}$ . For this partition the condition for lumpability is satisfied, see the exercises. This particular lumping would not have been possible for unequal probabilities of moving to left or right.

It is easy to verify that (see the exercises)

$$\begin{aligned}\hat{P} &= \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \end{pmatrix}, \\ \hat{N} &= \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix}, \\ \hat{\mathbf{w}} &= (3, 4)^T \\ \hat{B} &= (1, 1)^T.\end{aligned}$$

▽

**Example 12.12.** Let  $Q^k$  be the  $k$ -dimensional hypercube graph, with vertices or node set

$$V(Q^k) = \{x_0, x_1, \dots, x_{2^k}\} = \{0, 1\}^k$$

and edge set

$$E(Q^k) = \{(x, y) : x, y \text{ differ in one coordinate}\}.$$

A lazy random walk on this graph is the sequence  $X_0, X_1, \dots, X_{n-1}, X_n, \dots$  where, given  $X_n$ , first choose to remain at  $X_n$  with probability  $\frac{1}{2}$ . Alternatively, with probability  $\frac{1}{2}$  choose to move to  $X_{n+1}$  selected uniformly at random from the nodes adjacent to  $x_n$ . A practical way to implement this random walk is to choose a coordinate  $j \in \{1, 2, \dots, k\}$  uniformly at random and replace the bit in that position with the value of a fair Bernoulli random value. For example, on the 3-dimensional cube a walk at 011 will move to 111 with probability  $\frac{1}{2}$  or stay at 011 with probability  $\frac{1}{2}$  if coordinate 1 is selected, likewise to 001 or stay at 011 if coordinate 2 is selected, and 010 or stay at 011 if coordinate 3 is selected. As  $n \rightarrow \infty$ , the distribution of  $X_n$  converges to the uniform distribution  $\boldsymbol{\pi} = \frac{1}{2^k} \mathbf{1}$  on  $V(Q^k)$  (see the exercises). The aperiodic lazy random walk avoids the annoying issue of the usual random walk being periodic with period 2.

Next consider two urns labeled  $A$  and  $B$  which contain a total of  $k$  balls. In the alternate Ehrenfest urn model a ball is selected at random with all selections equally likely, and moved from the urn it is in to the other urn. The state at each time is the number of balls in the urn  $A$ , from 0 to  $n$ . Then the transition probability matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ \frac{1}{2k} & \frac{1}{2} & \frac{1}{2} - \frac{1}{2k} & 0 & \cdots & 0 & 0 \\ 0 & \frac{2}{2k} & \frac{1}{2} & \frac{1}{2} - \frac{2}{k} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \frac{1}{2k} \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}.$$

The balls fluctuate between the two containers with generally a drift from the one with the larger number of balls to the one with the smaller numbers.

The stationary distribution for this Markov chain has entry  $\pi_i = \binom{k}{i}/2^k$ . (See the exercises.) This is the binomial distribution on  $k$  with  $p = 1/2$ . For large  $k$ , the normal distribution approximates the stationary distribution.



The alternate Ehrenfest urn model is a lumping of the lazy random walk on the  $k$ -dimensional hypercube. A set  $E_\nu$  in the partition, that is, the equivalence class, is defined as the set of vertices with the sum of the coordinates equal to  $\nu \in \{0, 1, \dots, k\}$ . The position of the lazy random walk on the hypercube specifies the set of balls in urn  $A$ ; changing a bit corresponds to moving that particular ball into or out of the urn. See the exercises to prove this using the lumping condition theorem.

▽

### 12.7. Bounding Lumping Errors

Starting from a distribution  $x_0$  on  $\mathcal{X}$ , the time evolution of the distribution among the lumped states  $E_j$  is  $\hat{x}_t = x_0 P^t V$ , while the time evolution of the distribution of the lumped Markov chain is  $y_t = x_0 V \hat{P}^t$ . How different are these two dynamics?

For the following definition,  $\pi$  may be any properly sized vector, but later it will be chosen to be the stationary distribution vector. Define the norm  $\|\cdot\|_\pi$  by

$$\|v\|_\pi = \|v D_{\sqrt{\pi}}\|_2 = \sqrt{\sum_\nu v_\nu^2 / \pi_\nu}$$

where  $D_{\sqrt{\pi}} = \text{diag}(1/\sqrt{\pi_1}, \dots, 1/\sqrt{\pi_k})$  and  $\|\cdot\|_2$  is the standard Euclidean 2-norm. The corresponding operator norm is

$$\begin{aligned} \|A\|_\pi &= \max_{\|x\|_\pi=1} \|xA\|_\pi = \max_{\|x D_{\sqrt{\pi}}\|_2=1} \|x D_{\sqrt{\pi}} D_{\sqrt{\pi}}^{-1} A D_{\sqrt{\pi}}\|_2 = \\ &= \max_{\|w\|_2=1} \|w D_{\sqrt{\pi}}^{-1} A D_{\sqrt{\pi}}\|_2 = \|D_{\sqrt{\pi}}^{-1} A D_{\sqrt{\pi}}\|_2. \end{aligned}$$

Now using the  $v$ -dimensional stationary distribution vector  $\hat{\pi}$  on the lumped chain, the one step difference is

$$\|x_0 V \hat{P} - x_0 P V\|_{\hat{\pi}} = \|x_0 V U P V - x_0 P V\|_{\hat{\pi}} = \|x_0 (V U P - P) V\|_{\hat{\pi}}.$$

The  $n$  step difference is

$$\begin{aligned} \|x_0 V \hat{P}^n - x_0 P^n V\|_{\hat{\pi}} &= \|x_0 V (U P V)^n - x_0 P^n V\|_{\hat{\pi}} \\ &= \|x_0 V U P V U P V \dots U P V U P V - x_0 P^n V\|_{\hat{\pi}} = \\ &= \|x_0 (V U P)^n V - x_0 P^n V\|_{\hat{\pi}} = \|x_0 ((V U P)^n - P^n) V\|_{\hat{\pi}}. \end{aligned}$$

The important operator for bounding the difference is  $V U P$ . For convenience, let  $V U P = H$ .

The goal is to bound the  $n$  step difference  $\|H^n - P^n\|_\pi$  in terms of the 1-step difference  $\|H - P\|_\pi$  now using the right sized  $\pi$ . The general behavior of the difference is that it can at most grow for a while, but must eventually decline to 0 since by construction the lumped and unlumped chain converge to the same equilibrium distribution. Bounding how large the difference can get in terms of the 1 step difference is the next theorem.

**Theorem 12.13.** *Assume  $P$  is the transition probability matrix for an irreducible and aperiodic and reversible Markov chain. Let  $\delta = \|V U P - P\|_\pi$ . Then*

$$\|(V U P)^n - P^n\|_\pi \leq K(n) \delta \leq \hat{K} \delta$$

with  $K(n) = n|\lambda_2|^{n-1}$ , where  $\lambda_2$  is the second largest eigenvalue of  $P$  and  $\hat{K} = -1/(\lambda_2 \cdot e \cdot \log(\lambda_2))$ .

**Remark 12.14.** For further understanding, the matrices and projections used in the following proof are illustrated in the small case of the lumped weather example after the proof.

**Proof.** (1) First note that

$$\|H^n - P^n\|_{\pi} = \|(H - P)H^{n-1} + P(H^{n-1} - P^{n-1})\|_{\pi}.$$

(2) Iterating,

$$\begin{aligned} \|H^n - P^n\|_{\pi} &= \left\| \sum_{\nu=0}^{n-1} P^{\nu}(H - P)H^{n-\nu-1} \right\|_{\pi} \\ &\leq \sum_{\nu=0}^{n-1} \|P^{\nu}(H - P)H^{n-\nu-1}\|_{\pi}. \end{aligned}$$

(3) Recall that  $H$  and  $P$  have common stationary distribution  $\pi$ . Define the projection  $P_{\pi} = \mathbf{1}\pi$  where  $\mathbf{1}$  is an  $k \times 1$  column vector of 1s and  $\pi$  is the  $1 \times k$  stationary vector.  $P_{\pi}$  projects a column vector into the 1-dimensional subspace spanned by  $\mathbf{1}$ .

(4) The complementary projection is  $P_{\Sigma} = I - P_{\pi}$ .

(5) The decomposition into the subspaces gives the following representations of  $P$  and  $H$ :

$$\begin{aligned} P &= (P_{\pi} + P_{\Sigma})P = P_{\pi} + P_{\Sigma}P \\ H &= (P_{\pi} + P_{\Sigma})H = P_{\pi} + P_{\Sigma}H \end{aligned}$$

because  $P_{\pi}P = P_{\pi}$  and  $P_{\pi}H = P_{\pi}$  since the rows of  $P_{\pi}$  are the stationary vector  $\pi$ .

(6) Then  $H - P = P_{\Sigma}H - P_{\Sigma}P$  and  $0 = P_{\pi}P_{\Sigma}P = P_{\Sigma}PP_{\pi} = P_{\pi}P_{\Sigma}H = P_{\Sigma}HP_{\pi}$ .

(7) Recall  $\delta = \|VUP - P\|_{\pi}$  and  $VUP = H$ , so  $\|VUP - P\|_{\pi} = \|H - P\|_{\pi} = \|P_{\Sigma}H - P_{\Sigma}P\|_{\pi} = \delta$ .

(8) For integers  $\nu, n$

$$\begin{aligned} &\|P^{\nu}(H - P)H^{n-\nu-1}\|_{\pi} \\ &= \|(P_{\pi} + P_{\Sigma}P)^{\nu}(P_{\Sigma}H - P_{\Sigma}P)(P_{\pi} + P_{\Sigma}H)^{n-\nu-1}\|_{\pi} \\ &= \|(P_{\Sigma}P)^{\nu}(P_{\Sigma}H - P_{\Sigma}P)(P_{\Sigma}H)^{n-\nu-1}\|_{\pi} \\ &= \|P_{\Sigma}P\|_{\pi}^{\nu} \cdot \delta \cdot \|P_{\Sigma}H\|_{\pi}^{n-\nu-1}. \end{aligned}$$

(9) Use the special choice of norm, in particular, use the fact that for a matrix  $\|A\|_{\pi} = \|D_{\sqrt{\pi}}^{-1}AD_{\sqrt{\pi}}\|_2$ . By the assumption of reversibility,  $D_{\sqrt{\pi}}^{-1}PD_{\sqrt{\pi}}$  is a symmetric matrix. Therefore, the 2-norm is the dominant eigenvalue of the matrix. In fact, as shown below the diagonal matrix  $D_{\sqrt{\pi}}$  also symmetrizes  $P_{\pi}$  (see step 10),  $P_{\pi}P$  (see step 11),  $P_{\Sigma}P$  (see step 12), and  $VU$  (see steps 13 and 14). Therefore each has norm equaling the dominant eigenvalue.

(10) Direct calculation shows  $\pi D_{\sqrt{\pi}} = \mathbf{1}^T D_{\sqrt{\pi}}^{-1}$ . Starting with the definition of  $P_{\pi}$

$$\begin{aligned} D_{\sqrt{\pi}}^{-1} P_{\pi} D_{\sqrt{\pi}} &= D_{\sqrt{\pi}}^{-1} (\mathbf{1}\pi) D_{\sqrt{\pi}} = (\mathbf{1}^T D_{\sqrt{\pi}}^{-1})^T (\pi D_{\sqrt{\pi}}) = \\ &= (\pi D_{\sqrt{\pi}})^T (\pi D_{\sqrt{\pi}}) = ((\pi D_{\sqrt{\pi}})^T (\pi D_{\sqrt{\pi}}))^T = ((\mathbf{1}^T D_{\sqrt{\pi}}^{-1})^T (\pi D_{\sqrt{\pi}}))^T \\ &= ((D_{\sqrt{\pi}}^{-1} \mathbf{1})(\pi D_{\sqrt{\pi}}))^T = (D_{\sqrt{\pi}}^{-1} (\mathbf{1}\pi) D_{\sqrt{\pi}})^T = (D_{\sqrt{\pi}}^{-1} P_{\pi} D_{\sqrt{\pi}})^T. \end{aligned}$$

This shows  $P_{\pi}$  is symmetrized by  $D_{\sqrt{\pi}}$ .

(11) So  $D_{\sqrt{\pi}}^{-1} P D_{\sqrt{\pi}}$  and  $D_{\sqrt{\pi}}^{-1} P_{\pi} D_{\sqrt{\pi}}$  are symmetric and commute with each other since  $P$  and  $P_{\pi}$  commute. Thus,

$$D_{\sqrt{\pi}}^{-1} P_{\pi} P D_{\sqrt{\pi}} = D_{\sqrt{\pi}}^{-1} P_{\pi} D_{\sqrt{\pi}} D_{\sqrt{\pi}}^{-1} P D_{\sqrt{\pi}}$$

is symmetric.

(12) Then  $D_{\sqrt{\pi}}^{-1} P_{\Sigma} P D_{\sqrt{\pi}} = D_{\sqrt{\pi}}^{-1} (I - P_{\pi}) P D_{\sqrt{\pi}}$  is symmetric as well.

(13) From  $U_{ij} = V_{ji} \frac{\pi_j}{\sqrt{\pi_i}}$ , it follows that  $U = D_{\sqrt{\pi}}^2 V^T D_{\sqrt{\pi}}^{-2}$  so  $D_{\sqrt{\pi}}^{-1} U D_{\sqrt{\pi}} = D_{\sqrt{\pi}} V^T D_{\sqrt{\pi}}^{-1}$ .

(14) Thus,

$$\begin{aligned} D_{\sqrt{\pi}}^{-1} V U D_{\sqrt{\pi}} &= (D_{\sqrt{\pi}}^{-1} V D_{\sqrt{\pi}}) (D_{\sqrt{\pi}}^{-1} U D_{\sqrt{\pi}}) \\ &= (D_{\sqrt{\pi}}^{-1} V D_{\sqrt{\pi}}) (D_{\sqrt{\pi}} V^T D_{\sqrt{\pi}}^{-1}) \\ &= (D_{\sqrt{\pi}}^{-1} V D_{\sqrt{\pi}}) (D_{\sqrt{\pi}}^{-1} V D_{\sqrt{\pi}})^T. \end{aligned}$$

As the product of a matrix and its transpose,  $VU$  is symmetrized by  $D_{\sqrt{\pi}}$ .

(15) Since  $D_{\sqrt{\pi}}^{-1} P_{\Sigma} P D_{\sqrt{\pi}}$  is symmetric and using the definition of the matrix norm,  $\|P_{\Sigma} P\|_{\pi} = |\lambda_2|$ , where  $\lambda_2$  is the second-largest eigenvalue of  $P$ . To bound  $\|P_{\pi} H\|_{\pi}$ :

$$\begin{aligned} \|P_{\Sigma} H\|_{\pi} &= \|VUP - P_{\pi}\|_{\pi} = \|VUP - VUP_{\pi}\|_{\pi} \\ &= \|VU(P - P_{\pi})\|_{\pi} \leq \|P_{\Sigma} P\|_{\pi} \|VU\|_{\pi} = |\lambda_2| \|VU\|_{\pi}. \end{aligned}$$

(16) Since  $VU$  is a stochastic matrix and  $D_{\sqrt{\pi}}$  symmetrizes  $VU$ , it follows that  $\|VU\|_{\pi} = 1$ .

(17) Thus the bound becomes  $\|H^n - P^n\|_{\pi} \leq n |\lambda_2|^{n-1} \delta = K(n) \delta$  where  $K(n) = n |\lambda_2|^{n-1}$ .

(18) Maximizing  $K(n)$  over  $n$  gives  $K(n) \leq \hat{K} = \frac{-1}{\lambda_2 \cdot \log(\lambda_2)}$ .

□

**Corollary 12.15.**

$$\|x_0 V \hat{P}^n - x_0 P^n V\|_{\pi} \leq K_2 \cdot n |\lambda_2|^{n-1} \cdot \delta$$

where  $\delta = \|VUP - P\|_{\pi}$ ,  $\lambda_2$  is the second largest eigenvalue of  $P$  and  $K_2$  is a constant related to  $x_0$  and  $V$ .

**Proof.** See the exercises.

□

**Example 12.16.** For the weather example, the stationary distribution for  $P$  is  $(2/5, 1/5, 2/5)$  so the vector norm is

$$\|v\| = \sqrt{\frac{5v_1^2}{2} + 5v_2^2 + \frac{5v_3^2}{2}}$$

and the diagonalizing matrix is

$$D_{\sqrt{\pi}} = \begin{pmatrix} 1/\sqrt{2/5} & 0 & 0 \\ 0 & 1/\sqrt{1/5} & 0 \\ 0 & 0 & 1/\sqrt{2/5} \end{pmatrix}.$$

The transition probability matrix and the collecting and distributing matrices are

$$P = \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix}, \quad V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix}$$

so

$$H = VUP = \begin{pmatrix} 3/8 & 1/4 & 3/8 \\ 1/2 & 0 & 1/2 \\ 3/8 & 1/4 & 3/8 \end{pmatrix}.$$

The eigenvalues of  $P$  are 1,  $1/4$ , and  $-1/4$ . The stationary distribution for  $H$  is also  $(2/5, 1/5, 2/5)$  and the eigenvalues of  $H$  are 1, 0, and  $-1/4$ .

The projections are

$$P_{\pi} = \mathbf{1}\pi = \begin{pmatrix} 2/5 & 1/5 & 2/5 \\ 2/5 & 1/5 & 2/5 \\ 2/5 & 1/5 & 2/5 \end{pmatrix} \quad P_{\Sigma} = I - P_{\pi} = \begin{pmatrix} 3/5 & -1/5 & -2/5 \\ -2/5 & 4/5 & -2/5 \\ -2/5 & -1/5 & 3/5 \end{pmatrix}.$$

Although it is obvious by construction, directly verifying

$$P = (P_{\pi} + P_{\Sigma})P = P_{\pi} + P_{\Sigma}P$$

$$H = (P_{\pi} + P_{\Sigma})H = P_{\pi} + P_{\Sigma}H$$

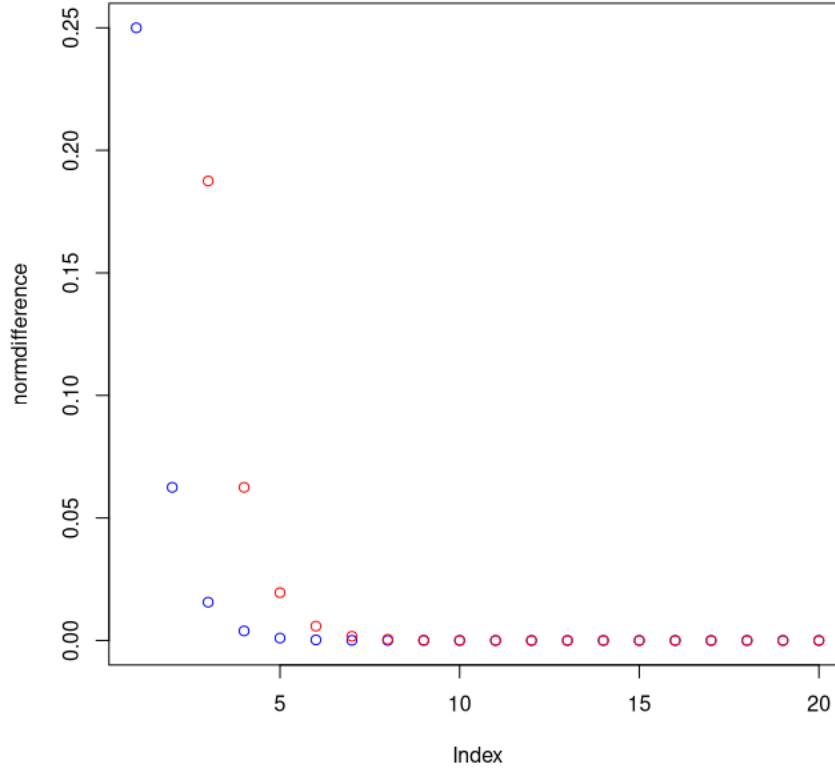
and  $H - P = P_{\Sigma}H - P_{\Sigma}P$  and  $0 = P_{\pi}P_{\Sigma}P = P_{\Sigma}PP_{\pi} = P_{\pi}P_{\Sigma}H = P_{\Sigma}HP_{\pi}$  is easy. Although it is obvious by construction, it is also easy to verify that  $D_{\sqrt{\pi}}^{-1}PD_{\sqrt{\pi}}$  is symmetric directly by computation. The diagonal matrix  $D_{\sqrt{\pi}}$  also symmetrizes  $P_{\pi}$ ,  $P_{\pi}P$ ,  $P_{\Sigma}P$ , and  $VU$ .

Figure 12.2 illustrates the numerical norm difference of the lumped chain with red dots from lumping the original chain with the blue points. The upper bound from the eigenvalue is illustrated with the red points, showing that the inequality is satisfied.

▽

## 12.8. Chapter Ending Answer

The probability of going from  $R$  to either  $R$  or  $S$  is  $\frac{1}{4} + \frac{1}{2} = \frac{3}{4}$ . The probability of going from  $S$  to either  $R$  or  $S$  is  $\frac{1}{2} + \frac{1}{4} = \frac{3}{4}$ . Any probability combination of being in the states  $R$  and  $S$  leads to a probability  $\frac{3}{4}$  of being in the states  $R$  or  $S$ , so the probability of going from bad weather to bad weather is  $\frac{3}{4}$ .



**Figure 12.2.** The numerical norm difference of the lumped chain from lumping the original chain in blue with the theoretical upper bound in red.

## 12.9. Chapter Summary

### Key Concepts.

- (1) Denote the transition probability of the Markov chain  $X_n$  from state  $x_i$  to state  $x_j$ , for  $i, j = 1, \dots, k$ , by  $P_{ij}$ . A necessary and sufficient condition for the Markov chain  $X_n$  to be lumpable with respect to the partition  $S$  is that for every pair of sets  $E_\xi$  and  $E_\eta$ ,  $\sum_{x_\nu \in E_\eta} P_{i,\nu}$  has the same value for every  $x_i \in E_\xi$ . These common values form the transition probabilities  $P_{\xi,\eta}$  for the lumped chain.
- (2) The **distributing matrix**  $U$  is the wide  $v \times k$  matrix with entries

$$U_{ij} = \begin{cases} \pi_j / \sum_{\nu \in E_j} \pi_\nu & x_j \in E_j \\ 0 & \text{otherwise.} \end{cases}$$

The rows of the distributing matrix are the stationary distribution restricted to  $E_j$  and renormalized so its entries add to 1. Let the **collecting matrix**  $V$

be the tall  $k \times v$  matrix with the  $j$ th column,  $j = 1, 2, \dots, v$ , is a vector with 1s in the components corresponding to states in  $E_j$ , and 0 elsewhere. The collecting matrix specifies the lumped probability distribution  $\hat{P} = PV$  on the partition  $E$ .

- (3) If  $P$  is the transition probability matrix of the Markov chain  $X_n$ , then  $X_n$  is lumpable with respect to the partition  $\mathcal{S}$ , if and only if  $VUPV = PV$ .
- (4) Let  $\delta = \|VUP - P\|_{\pi}$ . Then

$$\|(VUP)^n - P^n\|_{\pi} < K(n)\delta < \hat{K}\delta$$

with  $K(n) = n|\lambda_2|^{n-1}$ , where  $\lambda_2$  is the second largest eigenvalue of  $P$  and  $\hat{K} = -1/(\lambda_2 \cdot e \cdot \log(\lambda_2))$ .

### Vocabulary.

- (1) Let  $X_n$  be a Markov chain with state space  $\mathcal{X} = \{x_1, x_2, \dots, x_k\}$  and initial distribution  $X_0$ . Given a partition  $\hat{\mathcal{S}} = \{E_1, E_2, \dots, E_v\}$  of the state space  $\mathcal{S}$ , define a new stochastic process  $\hat{X}_n$  as follows: At the  $j$ th step, the state of the new chain is the set  $E_\ell$  when  $E_\ell$  contains the state of the  $j$ th step of the original chain. Assign the transition probabilities for  $\hat{X}_n$  as follows: The initial distribution is

$$\mathbb{P}[\hat{X}_0 = E_\xi] = \mathbb{P}_{X_0}[x_0 \in E_\xi].$$

Given the initial state, the transition probability for step 1 is

$$\mathbb{P}[\hat{X}_1 = E_\eta \mid \hat{X}_0 = E_\xi] = \mathbb{P}_{X_0}[X_1 \in E_\eta].$$

In general for the  $n$ th step

$$\begin{aligned} \mathbb{P}[\hat{X}_{n+1} = E_\eta \mid \hat{X}_n = E_{\eta_n}, \hat{X}_{n-1} = E_{\eta_{n-1}}, \dots, \hat{X}_1 = E_{\eta_1}, \hat{X}_0 = E_\xi] \\ = \mathbb{P}_{X_0}[X_{n+1} \in E_\eta \mid X_n \in E_{\eta_n}, X_{n-1} \in E_{\eta_{n-1}}, \dots, X_1 \in E_{\eta_1}, X_0 \in E_\xi]. \end{aligned}$$

Call this new stochastic process,  $\hat{X}_n$ , a **lumped chain** of the Markov chain  $X_n$ . Sometimes this is also called a *projection* of the Markov chain  $X_n$ .

- (2) A Markov chain  $X_n$  with state space  $\mathcal{X}$  is said to be **lumpable** with respect to a partition  $\hat{\mathcal{S}}$  of  $\mathcal{X}$  if for every starting distribution  $X_0$  the lumped process  $\hat{X}_n$  is a Markov chain with state space  $\hat{\mathcal{S}}$  and the associated transition probabilities do not depend on the choice of  $X_0$ .
- (3) The **distributing matrix**  $U$  is the  $v \times k$  matrix with entries

$$U_{ij} = \begin{cases} \pi_j / \sum_{\nu \in E_i} \pi_\nu & x_j \in E_i \\ 0 & \text{otherwise.} \end{cases}$$

The  $i$ th row of the distributing matrix is the stationary distribution restricted to  $E_i$  and renormalized so its entries add to 1.

- (4) Let the **collecting matrix**  $V$  be the  $k \times v$  matrix with the  $j$ th column,  $j = 1, 2, \dots, v$ , is a vector with 1 in the components corresponding to states in  $E_j$ , and 0 elsewhere. The collecting matrix specifies the lumped probability distribution  $\hat{p} = pV$  on the partition  $E$ .

- (5) Key theorems for irreducible and aperiodic Markov chains, absorbing Markov chains, and reversible Markov chains carry over to lumped Markov chains.

**Notation.**

- (1)  $X_n$  – discrete time, discrete space Markov chain
- (2)  $\mathcal{X} = \{x_1, x_2, \dots, x_k\}$  – state space
- (3)  $k$  – number of states in the Markov chain
- (4)  $x_i, x_j$  – generic states of Markov chain
- (5)  $P$  –  $k \times k$  transition probability matrix
- (6)  $p_{ij}$  – entry in the transition matrix
- (7)  $X_0$  – initial distribution or state of the Markov chain, with abuse of notation for the same notation to represent both an initial probability distribution over the states and the single state corresponding to a delta-distribution (certainty) on that state
- (8)  $\pi$  – stationary probability distribution
- (9)  $\hat{\mathcal{S}} = \{E_1, E_2, \dots, E_v\}$  – a partition of the state space  $\mathcal{X}$  into equivalence classes
- (10)  $v$  – number of states in the lumped chain
- (11)  $E_\xi, E_\eta$  – generic state of the lumped chain with  $E_\xi$  the source and  $E_\eta$  the destination.
- (12)  $\hat{X}_n$  – a lumped process
- (13)  $\hat{\pi}$  – lumped chain stationary distribution
- (14)  $U$  and  $V$  – distributing matrix and collecting matrix respectively
- (15)  $p, q$  – probability distributions on  $\mathcal{X}$
- (16)  $\hat{p}$  – corresponding probability distribution on  $\hat{\mathcal{S}}$
- (17)  $I_v$  –  $v \times v$  identity matrix
- (18)  $W_i$  – submatrices of  $VU$
- (19)  $I, R, Q$  – submatrices of absorbing chain transition probability matrix  $P$
- (20)  $U_1, U_2, V_1, V_2$  – submatrices of  $U, V$
- (21)  $\hat{N}, \hat{w}, \hat{B}$  – normal matrix and absorption quantities for lumped chain
- (22)  $Q^k, E(Q^k), V(Q^k)$  –  $k$ -dimensional hypercube as a graph, with the edge and vertex sets of the graph
- (23)  $\|v\|_\pi$  – vector norm related to  $\pi$
- (24)  $D_\pi$  – diagonal matrix with entries from  $\pi$
- (25)  $D_{\sqrt{\pi}}$  – diagonal matrix related to  $\pi$
- (26)  $H = VUP$  – matrix used for bounding norm difference
- (27)  $P_\pi, P_\Sigma$  – projection matrices
- (28)  $\Sigma$  – subspace complementary to span of  $\pi$
- (29)  $\delta$  – initial norm difference
- (30)  $\lambda_2$  – second largest eigenvalue

- (31)  $K(n), \hat{K}$  – upper bounds on norm difference
- (32)  $\nu$  – A dummy variable of summation, no meaning, meant to mimic the counting variable  $n$

### 12.10. Sources

The example of reducing the PageRank matrix is from Barreto and Fragoso.

The example of lumped chains from clustering or “communities” and the diagram are adapted from Piccardi.

The strategy of using the distributing and collecting matrices for lumped chains is adapted from [KS60].

The example of a lumped chain which is not Markov is adapted from class notes from Eric Slud, Statistics 650.

The accuracy bounds on the lumped chain are adapted from [HS09]

The example of lumping a random walk on the hypercube to the Ehrenfest urn model is based on Sections 2.3 of [LPW09].

### 12.11. Reading Suggestion:

### 12.12. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)



### 12.13. Algorithms and Scripts

**Data:** Transition probability matrix, collecting, distributing, diagonal matrices

**Result:** Plot of norm difference between lumped and original chain

- 1 *Initialization of Matrices*
- 2 Initialize  $P, V, U, D, Dinv$
- 3 Initialize  $\lambda_2$
- 4 Initialize number of iterations  $N$
- 5  $H \leftarrow VUP$
- 6  $H_n \leftarrow H$
- 7  $P_n \leftarrow P$
- 8  $normDifference \leftarrow [\|Dinv(H_n - P_n)D\|_2]$
- 9 **for**  $n \leftarrow 1$  **to**  $N - 1$  **do**
- 10      $H_n \leftarrow HH_n$
- 11      $P_n \leftarrow PP_n$
- 12     Append  $\|Dinv(H_n - P_n)D\|_2$  to  $normDifference$
- 13 **end**
- 14 Generate comparison list  $n\lambda_2^{n-1}$  for  $n = 1 : N$
- 15 Plot  $normDifference$  and comparison list on same axes

**Algorithm 15:** Illustration of Theorem 12.13.

**R:** R script for lumpedchains.R.

```

1 # Enter matrices by columns, the default in R
2 P <- matrix(c(1/2, 1/2, 1/4, 1/4, 0, 1/4, 1/4, 1/2, 1
   /2), nrow=3, ncol=3)
3 V <- matrix(c(0, 1, 0, 1, 0, 1), nrow=3, ncol = 2)
4 U <- matrix(c(0, 1/2, 1, 0, 0, 1/2), nrow=2, ncol=3)
5 D <- matrix(c(1/sqrt(2/5), 0, 0, 0, 1/sqrt(1/5), 0,
   0, 0, 1/sqrt(2/5)), nrow=3, ncol=3)
6 Dinv <- matrix(c(sqrt(2/5), 0, 0, 0, sqrt(1/5), 0, 0,
   0, sqrt(2/5)), nrow=3, ncol=3)
7
8 lambda2 <- 1/4
9
10 N <- 20
11 H <- V %*% U %*% P
12 Hn <- H
13 Pn <- P
14
15 normdifference <- c( norm( Dinv %*% (Hn - Pn) %*% D,
   type="2" ) )
16 for (n in 1:(N-1) ) {
17   Hn <- H %*% Hn
18   Pn <- P %*% Pn
19   normdifference <-

```

```

20         c( normdifference, norm( Dinv %*% (Hn - Pn) %*
21           % D, type="2") )
22     }
23   plot(normdifference, col="blue")
24   K <- function(n, l2) { n * l2^{n-1} }
25   points(K(1:N, lambda2), col="red")

```

## 12.14. Problems to Work for Understanding

Chapter 12: Lumped Markov Chains.

12.1: For the 5-state absorbing symmetric random walk with transition probability matrix

$$P = \begin{matrix} & \begin{matrix} s_1 & s_5 & s_2 & s_3 & s_4 \end{matrix} \\ \begin{matrix} s_1 \\ s_5 \\ s_2 \\ s_3 \\ s_4 \end{matrix} & \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 1/2 & 1/2 & 0 & 0 \end{pmatrix} \end{matrix}$$

and partition  $S = \{\{s_1, s_5\}, \{s_2, s_4\}, \{s_3\}\}$  show that the condition for lumpability is satisfied. Verify that

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

$$\hat{N} = \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix}$$

$$\hat{\mathbf{w}} = (3, 4)^T$$

$$\hat{B} = (1, 1)^T.$$

12.2: Show that for irreducible and aperiodic chains with  $\hat{\pi} = \pi V$

$$U_{ij} = V_{ji} \frac{\pi_j}{\pi_i}, \quad i = 1, \dots, k, j = 1, \dots, v$$

whose  $i$ th row,  $i = 1, 2, \dots, v$ , is the probability vector having equal values for states in  $E_\xi$  and 0 elsewhere.

12.3: For the lazy random walk  $X_n$  on the hypercube  $Q^k$  show that as  $n \rightarrow \infty$ , the distribution of  $X_n$  converges to the uniform distribution  $\pi$  on  $V(Q^k)$ .

12.4: Prove that the stationary distribution for the alternate Ehrenfest urn model has entry  $\pi_i = \binom{k}{i}/2^k$ .

12.5: Show the alternate Ehrenfest urn model is a lumping of the lazy random walk on the  $n$ -dimensional hypercube using the correspondence between  $\{0, 1\}^n$  and subsets of  $\{0, 1, \dots, n\}$ , under which a vertex corresponds to the vector or bit string with 1s in the positions of its elements. The position of the random walk on the hypercube specifies the set of balls in urn  $A$ ; changing a bit corresponds to moving that numbered ball into or out of the urn.

12.6: For the lumping of the lazy random walk on the 3-dimensional cube  $Q^3$  starting at the origin into the alternate Ehrenfest urn model with 3 balls, plot the norm-difference of the distribution of the Ehrenfest urn model from the distribution of the lumped random walk and compare to the theoretical upper bound.

12.7: (1) For the weather in Oz with the distribution  $p = (1/6, 1/12, 3/4)$  on  $\{R, N, S\}$ , the lumped distribution  $\{G, B\}$  is  $\hat{p} = pV = (1/12, 11/12)$ . Calculate  $\|pV\|_{\hat{\pi}}$  and  $\|p\|_{\pi}$ .

(2) Show in general that for any irreducible and aperiodic Markov chain and any distribution  $\|pV\|_{\hat{\pi}} \leq \|p\|_{\pi}$ .

12.8: Show

$$\|x_0 V \hat{P}^n - x_0 P^n V\|_{\hat{\pi}} \leq K_2 \cdot n |\lambda_2|^{n-1} \cdot \delta$$

where  $\delta = \|VUP - P\|_{\pi}$ ,  $\lambda_2$  is the second largest eigenvalue of  $P$  and  $K_2$  is a constant related to  $x_0$ .

---

*Part 2*

## **Advanced Examples and Theory**



## Motivational Examples for the Metropolis Algorithm

### 13.1. Rating

The purpose of this chapter is to provide motivational examples of the Metropolis algorithm for creating Markov chains which converge to a given distribution. These examples are from group theory, and statistical mechanics. The examples and results are presented without proofs. These examples range from simple to sophisticated Markov chains.

Mathematicians Only: prolonged scenes of intense rigor.

### 13.2. Chapter Starter Question

- (1) What is the “cycle and transposition” notation for elements of the group of permutations on  $n$  elements?
- (2) Explain an algorithm for selecting a random permutation from the group of permutations on  $n$  elements.

### 13.3. Symmetric Function Theory

Let  $\mathcal{X} = S_n$ , the **symmetric group** of  $n$  letters, that is, the group of permutations on  $n$  letters.

**Remark 13.1.** This section uses the following notation for specific elements of  $S_n$ . For compact but complete representation, a permutation will usually be a row vector or ordered list with square brackets. For example in  $S_6$  the permutation  $[3, 4, 5, 6, 1, 2]$  is the function which carries the letter in position 1 to position 3, the letter in position 2 to position 4 and so on to the letter in position 6 carried to position 2. This is an “active permutation” in the sense used by Hankin [?] and

takes less space than the matrix format

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 4 & 5 & 6 & 1 & 2 \end{pmatrix}.$$

Hankin refers to this format as a permutation in “word” format. The classic representation of permutations in terms of cycles is also necessary in this section. The example permutation would be written as  $(1, 3, 5)(2, 4, 6)$  with parentheses around the cycles. Hankin refers to this as the cycle representation. Transpositions are the short cycles  $(i, j)$  and cycles leaving an element fixed are  $(i)$ .

The group operation is composition of permutations, thinking of them as functions, written with a small circle. The symmetric group element  $\sigma \circ \tau$  is the function applying  $\sigma$ , and then applying function  $\tau$ . For example, the first entry in the word representation of  $\sigma \circ \tau$  is  $\tau(\sigma(1))$ . Postfix notation for the functions would denote the action of the permutation on letter or position  $x$  as  $x\sigma\tau$ .

Let  $d(\sigma, \sigma_0)$  be a metric on the symmetric group by

$$\begin{aligned} d(\sigma, \sigma_0) &= \text{minimum number of transpositions to bring } \sigma \text{ to } \sigma_0 \\ &= \text{minimum number of transpositions in a representation of } \sigma^{-1} \circ \sigma_0. \end{aligned}$$

This metric is called **Cayley’s distance** because a result of A. Cayley implies that  $d(\sigma, \sigma_0) = n - \text{cycles}(\sigma^{-1} \circ \sigma_0)$  where  $\text{cycles}(\tau)$  is the number of cycles, including fixed cycles, in  $\tau \in S_n$ . This metric is bi-invariant:  $d(\sigma, \sigma_0) = d(\tau \circ \sigma, \tau \circ \sigma_0) = d(\sigma \circ \tau, \sigma_0 \circ \tau)$ . Later  $\sigma_0$  will be a distinguished or central element, usually the identity, so the metric measures distances from this “center”.

**Example 13.2.** In  $S_6$ , let  $\sigma_0 = [3, 4, 5, 6, 1, 2] = (1, 3, 5)(2, 4, 6)$ . Consider  $\sigma = [2, 6, 4, 3, 1, 5] = (1, 2, 6, 5)(3, 4)$ . The permutation that carries  $\sigma$  to  $\sigma_0$  is  $[1, 3, 6, 5, 2, 4] = (1)(2, 3, 6, 4, 5)$ . Writing

$$(2, 3, 6, 4, 5) = (2, 3)(3, 6)(6, 4)(4, 5) = (2, 5)(2, 4)(2, 6)(2, 3),$$

the minimum number of transpositions that brings  $\sigma$  to  $\sigma_0$  is 4 so  $d(\sigma, \sigma_0) = 4$ . Furthermore,  $\sigma^{-1} = [5, 1, 4, 3, 6, 2]$  so (remembering how permutations are functions)  $\sigma^{-1} \circ \sigma_0 = [1, 3, 6, 5, 2, 4] = (1)(2, 3, 6, 4, 5)$  with 2 cycles. This is an example of Cayley’s theorem that  $d(\sigma, \sigma_0) = n - \text{cycles}(\sigma^{-1} \circ \sigma_0) = 6 - 2 = 4$ .  $\nabla$

**Example 13.3.** As another larger example, consider  $S_{11}$  with

$$\sigma_0 = [4, 2, 9, 10, 6, 5, 11, 7, 8, 1, 3] = (1, 4, 10)(3, 9, 8, 7, 11)(5, 6).$$

Take  $\sigma = [7, 4, 5, 3, 1, 2, 11, 9, 8, 6, 10]$ . The permutation that carries  $\sigma$  to  $\sigma_0$  is

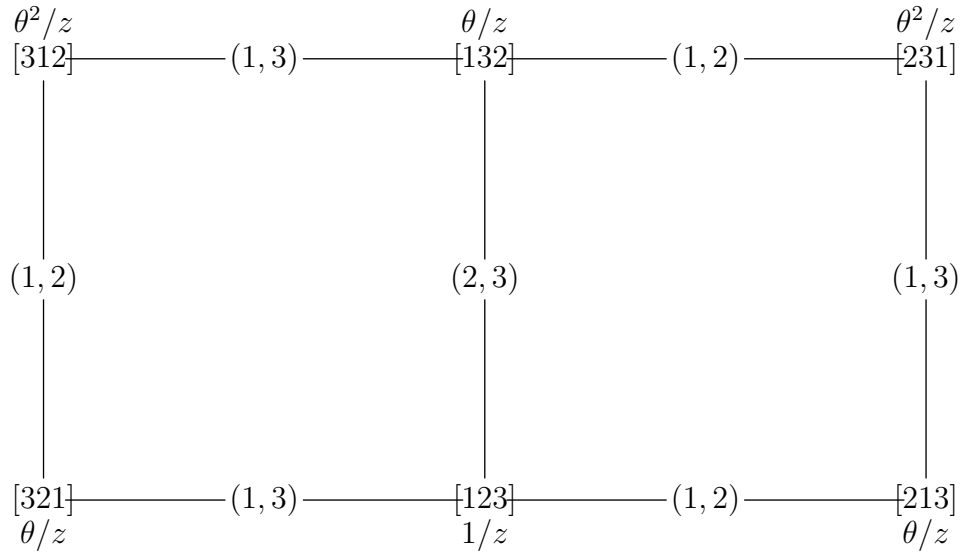
$$\begin{aligned} [6, 5, 10, 2, 9, 1, 4, 8, 7, 3, 11] &= (1, 6)(2, 5, 9, 7, 4)(3, 10)(8, 11) \\ &= (1, 6)(2, 5)(5, 9)(9, 7)(7, 4)(3, 10). \end{aligned}$$

The minimum number of transpositions that brings  $\sigma$  to  $\sigma_0$  is 6 so  $d(\sigma, \sigma_0) = 6$ . Furthermore,

$$\sigma^{-1} = [5, 6, 4, 2, 3, 10, 1, 9, 8, 11, 7] = (1, 5, 3, 4, 2, 6, 10, 11, 7)(8, 9)$$

so (remembering that permutations are functions)

$$\sigma^{-1} \circ \sigma_0 = [6, 5, 10, 2, 9, 1, 4, 8, 7, 3, 11] = (1, 6)(2, 5, 9, 7, 4)(3, 10)(7, 9)$$



**Figure 13.1.** The graph of  $S_3$  with transpositions indicated on the edges, giving a diagram of the metric space with the metric being the number of edges between any two permutations and the probability distribution above and below each permutation.

with 5 cycles. This is an example of Cayley's theorem that  $d(\sigma, \sigma_0) = n - \text{cycles}(\sigma^{-1} \circ \sigma_0) = 11 - 5 = 6$ .  $\nabla$

Fix  $\sigma_0$ , usually the identity permutation  $\sigma_0 = \text{id}$ . Define a probability distribution on  $S_n$  by

$$\mathbb{P}([\cdot] \mid \sigma) = z^{-1} \theta^{d(\sigma, \sigma_0)}, \sigma, \sigma_0 \in S_n, 0 < \theta \leq 1.$$

The normalizing constant is known in this example:

$$z = \sum_{\sigma} \theta^{d(\sigma, \sigma_0)} = \prod_{\nu=1}^n (1 + (\nu - 1)\theta).$$

If  $\theta = 1$ , then  $p(\sigma)$  is the uniform distribution on  $S_n$ . For  $0 < \theta < 1$ ,  $p(\sigma)$  is largest at  $\sigma_0$  and falls off from its maximum as  $\sigma$  moves away from  $\sigma_0$ . This becomes a nonuniform distribution on  $S_n$ , with the distribution having a peak at  $\sigma_0$ . An example with the small permutation group  $S_3$  is illustrated in Figure 13.1 with the metric being the number of edges between any two permutations. The normalizing constant is  $z = 1 + 3\theta + 2\theta^2 = (1)(1 + \theta)(1 + 2\theta)$ .

The main problem here is “How can samples be drawn from this distribution  $\mathbb{P}[\cdot]$  defined on the symmetric group?” The answer here is to use a Markov chain defined by the Metropolis algorithm, based on random transpositions. To be specific, moving from  $\sigma$ , choose a transposition  $(i, j)$  uniformly at random and consider  $(i, j)\sigma = \sigma^*$ . If  $d(\sigma^*, \sigma_0) \leq d(\sigma, \sigma_0)$  the Markov chain state moves to  $\sigma^*$ . If  $d(\sigma^*, \sigma_0) > d(\sigma, \sigma_0)$ , flip a coin with probability  $\theta$  of coming up heads. If the coin comes up heads, move to  $\sigma^*$ , otherwise stay at  $\sigma$ . The Markov chain transition



probabilities are

$$P(\sigma, \sigma^*) = \begin{cases} 1/\binom{n}{2} & \sigma^* = (i, j)\sigma, \quad d(\sigma^*, \sigma_0) \leq d(\sigma, \sigma_0) \\ \theta/\binom{n}{2} & \sigma^* = (i, j)\sigma, \quad d(\sigma^*, \sigma_0) > d(\sigma, \sigma_0) \\ (1 - m\theta)/\binom{n}{2} & \sigma^* = \sigma, \quad m = \text{card}(\{(i, j) : d((i, j)\sigma, \sigma_0) > d(\sigma, \sigma_0)\}) \\ 0 & \text{otherwise} \end{cases}.$$

This Markov chain usually moves toward  $\sigma_0$ , with occasional steps away from  $\sigma_0$ . This is consistent with the nonuniform distribution on  $S_n$ , with the distribution having a peak at  $\sigma_0$ . The Metropolis construction guarantees the stationary distribution  $\pi$  of this Markov chain is the distribution  $\mathbb{P}[\cdot]$ . Note that this discrete state space and discrete time Markov chain is a specific example of a random walk on the graph in Figure 13.1.

When  $n = 3$ ,  $\mathcal{X} = S_3$  and  $\sigma_0 = \text{id} = [123]$  the complete transition probability matrix is (see the exercises)

$$\begin{array}{c} [123] \quad [213] \quad [321] \quad [132] \quad [231] \quad [312] \\ \begin{array}{c} [123] \\ [213] \\ [321] \\ [132] \\ [231] \\ [312] \end{array} \begin{pmatrix} 1 - \theta & \frac{\theta}{3} & \frac{\theta}{3} & \frac{\theta}{3} & 0 & 0 \\ \frac{1}{3} & \frac{2}{3}(1 - \theta) & 0 & 0 & \frac{\theta}{3} & \frac{\theta}{3} \\ \frac{1}{3} & 0 & \frac{2}{3}(1 - \theta) & 0 & \frac{\theta}{3} & \frac{\theta}{3} \\ \frac{1}{3} & 0 & 0 & \frac{2}{3}(1 - \theta) & \frac{\theta}{3} & \frac{\theta}{3} \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \end{pmatrix} \end{array}.$$

The stationary distribution is the left eigenvector proportional to  $(1, \theta, \theta, \theta, \theta^2, \theta^2)$ , precisely the distribution  $\mathbb{P}[\cdot]$ . So sampling from the distribution  $\mathbb{P}[\cdot]$  can be done by running the Markov chain long enough and using the resulting distribution of states. The eigenvalues are  $1, \frac{2}{3}(1 - \theta), -\theta, 0$  with multiplicities 1, 1, 3 and 1 respectively

A theorem from Diaconis [DS81, Dia09, DS98], shows that starting from the identity and using the identity as  $\sigma_0$ , on the order of  $n \log n$  steps are necessary and sufficient to make the distance to stationarity small. If the chain starts far from the identity, for example at an  $n$ -cycle, it can be shown that order  $n^2 \log n$  steps suffice. In the example for  $S_3$  this means between 3 to 10 steps. As a larger example, if  $n = 52$ , the number of cards in a standard deck, then  $n \log n \approx 205.465$ , while  $n^2 \log n \approx 10684.163$ . So the running time for sampling from the stationary distribution should be from about several hundred to several tens of thousands of steps.

### 13.4. General Setting from Statistical Mechanics

The following is a general setting of Markov chains in statistical mechanics with some illustrative examples. A more specific model is described in detail in the next section.

A state of the multiple particles in the statistical mechanical model is described by a **configuration**  $x$  from the state space  $\mathcal{X}$ , called a **configuration space** in statistical mechanics. The configuration space can be infinite or finite, continuous or discrete. For example, with  $N$  interacting particles, each particle's position and

velocity in three-dimensional space specifies a configuration. In this case,  $\mathcal{X}$  is an infinite, continuous subset of  $\mathbb{R}^{6N}$ . As another example,  $\mathcal{X}$  might be taken as a bounded subset  $\Lambda$  of the integer lattice in the plane, attaching a value  $\pm 1$  to each site in  $\Lambda$ . This value might indicate the presence of particle there, or it might indicate an orientation (or spin) of a particle at the site. If  $\text{card}(\Lambda) = N$ , then the configuration space  $\mathcal{X}$  consists of all  $2^N$  possible assignments of values to sites in  $\Lambda$ .

The physics of a configuration space  $\mathcal{X}$  is described by an energy function  $E : \mathcal{X} \rightarrow \mathbb{R}^+$ . The energy of a particular configuration is  $E(x)$ . For the continuous example, the energy could be the sum of potential energies, or the sum of all kinetic energies, or the sum of both. For the discrete example above, the energy could show the total influence that neighboring particles exert on each other. This is the **Ising** model. Note that the configuration space and the number of states is quite large compared with most of the standard examples of Markov chains.

A basic principle of statistical physics is that Nature prefers low-energy configurations with high probability. This principle governs the random organization of molecules in a room. Rarely observed configurations, say all the molecules gathering in a corner of the room have high energies and hence low probabilities. In fact, the probabilities are so low such configurations are in principle never observed. Common configurations, such as all molecules distributed uniformly at all locations throughout the room have low energies and hence higher probabilities, high enough that those configurations are essentially the only configurations ever observed.

For a system at equilibrium, the relative frequency of a configuration  $x$  is given by its **Boltzmann weight**

$$e^{E(x)/kT}$$

where  $T$  is the temperature and  $k$  is Boltzmann's constant. For any  $x \in \mathcal{X}$ , its Boltzmann probability  $\text{Boltz}(x)$  is

$$\text{Boltz}(x) = \frac{e^{E(x)/kT}}{z}$$

where the denominator

$$z = \sum_{x \in \mathcal{X}} e^{E(x)/kT}$$

is called the **partition function**. In any realistic setting, the partition function is analytically and computationally intractable. This intractability accounts for the scarcity of analytic, closed-form results in statistical mechanics.

The total energy of the system is the expected value of the energy function, defined by

$$\langle E \rangle = \sum_{x \in \mathcal{X}} E(x) \text{Boltz}(x) = \frac{\sum_{x \in \mathcal{X}} E(x) e^{E(x)/kT}}{z}.$$

Other physical properties are defined similarly. In each case, there is no avoiding the partition function  $z$ .

Expressions such as the total energy could be naively approximated by using simple sampling. Generate a sample  $x_1, x_2, \dots, x_M$  *uniformly* from  $x$  and estimate

both the numerator and the denominator separately, giving

$$\langle E \rangle \approx \frac{\sum_{\nu=1}^M E(x_\nu) e^{E(x_\nu)/kT}}{\sum_{\nu=1}^M e^{E(x_\nu)/kT}}.$$

The limitation of sampling uniformly from the configuration space is not practical since a configuration where  $e^{E(x)/kT}$  is very small gets chosen with high probability; that is a configuration with low weight. The key to the Metropolis algorithm is that instead of choosing configurations randomly, then weighting them with  $e^{E(x)/kT}$ , instead choose configurations with probability  $e^{E(x)/kT}$  and weight them uniformly. In other words, it is better to sample from  $\mathcal{X}$  so that  $x$  is selected with probability Boltz( $x$ ). If this can be done, then for any such sample  $x_1, x_2, \dots, x_M$

$$\frac{1}{M} \sum_{\nu=1}^M E(x_\nu) \rightarrow \langle E \rangle$$

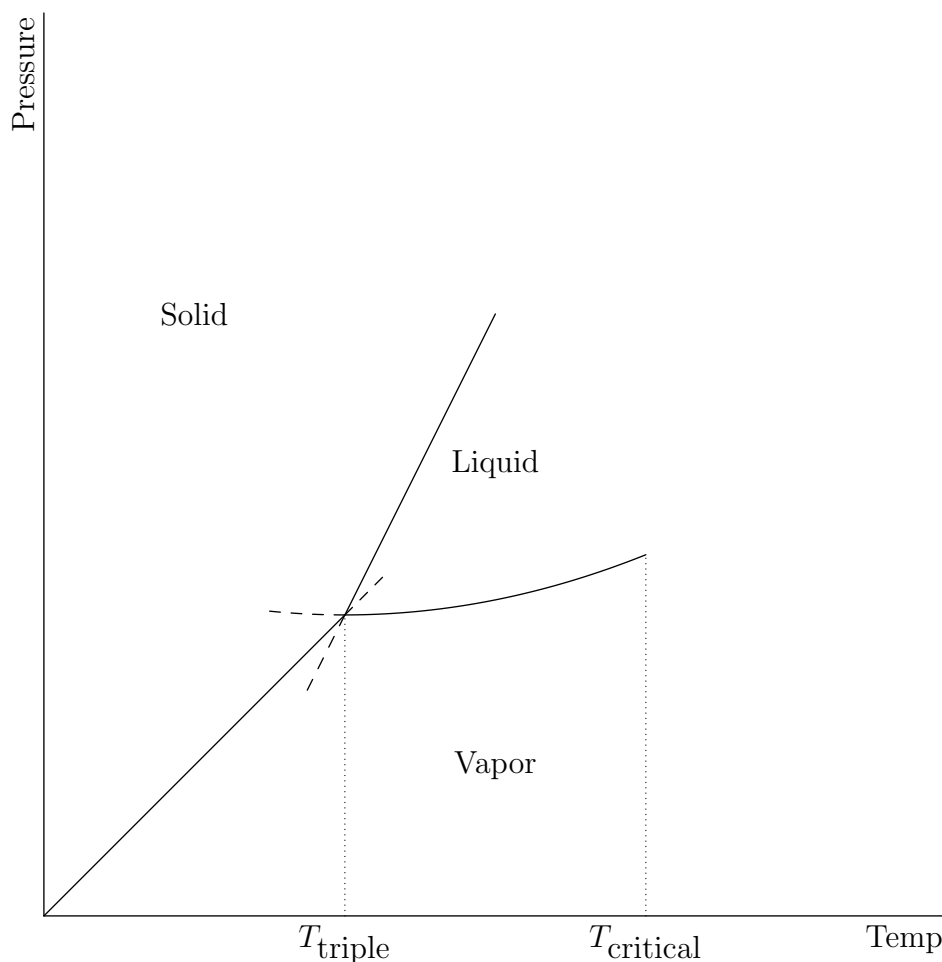
as  $M \rightarrow \infty$  with rate of convergence  $O(M^{-1/2})$ . The challenge is to sample from the nonuniform distribution.

### 13.5. Phase Transitions and Hard Disks

The study of phase transitions in statistical mechanics is a classical problem. For many substances, like water, experiments produce phase diagrams such as that shown in the schematic Figure 13.2. The general picture has a finite length liquid-vapor phase transition line ending in a critical point and a triple point of temperature and pressure where all three forms of matter coexist. A solid-liquid phase line extends to infinity. This general form of the phase transition diagram seems universal for all kinds of matter. This suggests there must be a general explanation, independent of details such as molecular structure. As a model, the physicist John G. Kirkwood posed the problem of whether a gas of hard spheres would show phase transitions.

As a simplified two-dimensional hard spheres model consider placement of  $n$  discs of radius  $\epsilon$  in the unit square. The discs must be non-overlapping and completely contained in the unit square. Typically,  $n$  is large on the order of 100 to  $10^6$  with  $\epsilon$  correspondingly small. The centers of the discs give a configuration point in the configuration space,  $[0, 1]^{2n}$ . Consider the set of configurations  $\mathcal{X}(n, \epsilon)$  for fixed  $n$ . One can think of the configuration as something like a “foam” in  $[0, 1]^{2n}$ . For fixed  $n$  and  $\epsilon$  very small this set is connected, one can move from one point in  $\mathcal{X}(n, \epsilon)$  to another point by sliding one or more discs around in the square. Some points in  $[0, 1]^{2n}$  will be inaccessible because the corresponding discs overlap or extend outside the square. By its embedding in  $[0, 1]^{2n}$ ,  $\mathcal{X}(n, \epsilon)$  inherits a natural uniform distribution, Lebesgue measure restricted to  $\mathcal{X}(n, \epsilon)$ . The problem is to pick points in  $\mathcal{X}(n, \epsilon)$  uniformly. Choosing  $X_1, X_2, \dots, X_M$  with uniform distribution for function  $f : \mathcal{X}(n, \epsilon) \rightarrow \mathbb{R}$  gives the approximation

$$\int_{\mathcal{X}(n, \epsilon)} f(x) \, dx \approx \frac{1}{M} \sum_{\nu=1}^M f(X_\nu).$$



**Figure 13.2.** Schematic phase transition diagram.

This hard disks problem is the original motivation for the Metropolis algorithm. The following is a version of the Metropolis algorithm for hard discs.

- (1) Start with a configuration  $x \in \mathcal{X}(n, \epsilon)$ .
- (2) Pick a disc in that configuration at random, that is, with probability  $1/n$ .
- (3) Pick a point at random in a disc of radius  $h$ , centered at the chosen disc center.  
At random means with Lebesgue measure restricted to the disc of radius  $h$ .
- (4) Try to move the chosen disc center to the chosen point, if the resulting configuration is in  $\mathcal{X}(n, \epsilon)$  accept the move; else, stay at  $x$ .
- (5) The algorithm continues, randomly moving coordinates.

The algorithm provides a discrete time continuous space Markov chain. If  $X_1, X_2, \dots, X_M$  are successive configurations, then theory and simulations show that  $X_M$  becomes

uniformly distributed provided  $\epsilon$  is small and  $M$  is large. For large  $M$ , the  $X_i$  can be used to approximate integrals as above.

This hard disks model has been studied from a number of perspectives. Simulations indicate a phase transition when the density of disks is about 0.71. This empirical value is below the close packing density which is  $\frac{\pi\sqrt{3}}{6} \approx 0.9069$ . Below the transition density, the disks look random, above the transition density, the disks look close to a lattice packing. The notions of randomness and packing are quantified by a variety of functions. For example,

$$f(x) = \left| \frac{1}{n} \sum_{\nu=1}^n \frac{1}{n_\nu} \sum_{\ell} e^{6i\theta_{\nu,\ell}} \right|$$

where the sum is over the  $n$  particles encoded by  $x \in [0, 1]^{2n}$ , the sum in  $\ell$  is over the  $n_\ell$  neighbors of the  $\nu$ th particle and  $\theta_{\nu,\ell}$  is the angle between the particles  $\nu$  and  $\ell$  in some fixed reference frame. If the configuration has a local hexagonal structure, the sum should be small. Different functions can be used to study long-range order.

### 13.6. A Generalization of Hard Disks

Let  $\mathcal{X} \subset \mathbb{R}^d$  be a bounded connected open set. Let  $\tilde{p}(x) > 0$ ,  $z = \int_{\mathcal{X}} \tilde{p}(x) \, dx < \infty$ ,  $\mathbb{P}[x] = z^{-1}\tilde{p}(x)$  be a probability distribution on  $\mathcal{X}$ . As necessary, extend  $p(x) = 0$  outside  $\mathcal{X}$ , the topological closure of  $\mathcal{X}$ . Sampling problems can be stated as *Given  $\tilde{p}$ , choose points in  $\mathcal{X}$  from  $\mathbb{P}[\cdot]$* . Note that the normalizing constant  $z$  may not be given and is usually impossible to approximate. As an example, consider placing fifty hard discs of radius  $\epsilon = 1/100$  randomly in the unit square. The set of allowable configurations is a complex “cuspy” set. Even though  $\tilde{p} = 1$  on  $\mathcal{X}$ , it is not practical to compute  $z$ . Nevertheless, it is still possible to sample from  $\mathbb{P}[\cdot]$ .

- (1) For  $x \in \mathcal{X}$ , fix a small positive  $h$ .
- (2) Choose  $y \in B_x(h)$ , from normalized Lebesgue measure on the ball  $B_x(h) \subset \mathbb{R}^d$ .
- (3) If  $\mathbb{P}[y] \geq \text{Prob}x$ , move to  $y$ .
- (4) If  $\mathbb{P}[y] < \mathbb{P}[x]$ , move to  $y$  with probability  $\mathbb{P}[y] / \mathbb{P}[x]$ .
- (5) If  $\mathbb{P}[y] < \mathbb{P}[\cdot](x)$ , stay at  $x$  with probability  $1 - \mathbb{P}[y] / \mathbb{P}[x]$ .

Note that this algorithm does not require knowing  $z$  because it only relies on the ratio  $\mathbb{P}[y] / \mathbb{P}[x] = \tilde{p}(y) / \tilde{p}(x)$ . The transition from  $x$  to  $y$  has a transition kernel (not matrix, since the state space is continuous)

$$P(x, dy) = m(x)\delta_x + \frac{h^{-d}}{\text{Vol}(B_1)}\delta_{B_1}\left(\frac{x-y}{h}\right) \min\left(\frac{p(x)}{p(y)}, 1\right) dy$$

where

$$m(x) = 1 - \int_{\mathbb{R}^d} \frac{h^{-d}}{\text{Vol}(B_1)}\delta_{B_1}\left(\frac{x-y}{h}\right) \min\left(\frac{p(x)}{p(y)}, 1\right) dy.$$

This kernel operates on  $L^2(p)$  by

$$P[f](x) = \int_{\mathbb{R}^d} f(y)P(x, dy).$$

$P(x, dy)$  is a bounded self-adjoint operator on  $L^2(p)$ . Describe this discrete time continuous space Markov chain as:

- (1) Start at  $X_0 = x \in \mathcal{X}$ .
- (2) Pick  $X_1$  from  $P(X_0, dy)$ .
- (3) Pick  $X_2$  from  $P(X_1, dy)$ .
- (4) Continue this process.

This means that

$$P(X_2 \in A) = P_x^2(A) = \int_{\mathbb{R}^d} P(z, A)P(x, dz),$$

and more generally

$$P(X_M \in A) = P_x^M(A) = \int_{\mathbb{R}^d} P(z, A)P^{M-1}(x, dz).$$

Under the assumptions that for  $\mathcal{X}$  connected and  $h$  small, then for all  $x \in \mathcal{X}$  and  $A \subset \mathcal{X}$ , the process converges to the stationary distribution,

$$P_x^M(A) \rightarrow \int_A p(y) dy.$$

A natural question is to ask how fast this convergence occurs. How many steps should the algorithm be run to achieve an acceptable degree of convergence? The following theorem of Diaconis, Lebeau and Michel gives an estimate:

**Theorem 13.4** (Diaconis, Lebeau, Michel). *Let  $\mathcal{X}$  be a connected Lipschitz domain in  $\mathbb{R}^d$ . For  $p$  measurable (with  $0 < m \leq p(x) \leq M < \infty$  on  $\mathcal{X}$ ) and  $h$  fixed and small, the Metropolis algorithm satisfies*

$$\left| P_x^M(A) - \int_A p(y) dy \right| \leq c_1 e^{-c_2 M h^2} \text{ uniformly in } x \in \mathcal{X}, A \subset \mathcal{X}.$$

Here  $c_1, c_2$  are positive constants that depend on  $\tilde{p}$  and  $\mathcal{X}$  but not on  $x, M$  or  $h$ . The inequality has a matching lower bound. Good estimates on  $c_2$  are available.

Note that the Metropolis algorithm in this section is based on steps in the full-dimensional ball  $B_{\epsilon(x)}$  while the Metropolis algorithm for discs in the previous section is based on changing just two coordinates at a time.

### 13.7. Chapter Ending Answer

- (1) The cycle  $(i_1, i_2, \dots, i_r)$  is the permutation that sends element  $i_1$  to  $i_2$ ,  $i_2$  to  $i_3$  and so on, until  $i_r$  is sent to  $i_1$ , leaving all other elements fixed. A transposition is just a 2-cycle  $(i_1, i_2)$  exchanging 2 elements. Compose cycles by composing the permutations each represents. A standard result about permutations is that every permutation is the composition of its cycles, and that every permutation is uniquely expressed as the composition of its disjoint cycles. Furthermore, a simple examination shows that the cycle  $(i_1, i_2, \dots, i_r)$  can be written as  $(i_1, i_2)(i_1, i_3) \dots (i_1, i_r)$  so that every cycle can be written as the product of transpositions.

- (2) A simple algorithm to generate a permutation of  $n$  items uniformly at random without retries, known as the Knuth shuffle or the modern Fisher-Yates algorithm, is to start with any permutation (for example, the identity permutation), and then go down through the positions  $n$  to 1. For each position  $i$  swap the element currently there with a randomly chosen element from positions 1 through  $i$  inclusive. It follows that this algorithm will produce any permutation of  $n$  elements with probability exactly  $1/n!$ , thus yielding a uniform distribution over all such permutations.

### 13.8. Chapter Summary

#### Key Concepts.

- (1) Let  $X = S_n$ , the **symmetric group** of  $n$  letters, that is, the set of permutations on  $n$  letters with the Cayley distance as metric. The metric defines a probability distribution on  $S_n$  by

$$\pi(\sigma) = z^{-1} \theta^{d(\sigma, \sigma_0)}, \sigma, \sigma_0 \in S_n, 0 \leq \theta \leq 1.$$

Choose a transposition  $(i, j)$  uniformly at random and consider  $(i, j)\sigma = \sigma^*$ . Using the Metropolis algorithm with this transposition defines a Markov chain on the symmetric group. A theorem from Diaconis [DS98, DS81] shows that starting from the identity and using the identity as  $\sigma_0$ , on the order of  $n \log n$  steps are necessary and sufficient to make the distance to the stationary distribution  $\pi$  small.

- (2) A state of the particles in statistical mechanics is described by a **configuration**  $\omega$  from the **configuration space**  $\Omega$ . The physics of a configuration space  $\Omega$  is described by an energy function  $E : \Omega \rightarrow \mathbb{R}^+$ . A basic principle of statistical physics is that Nature seeks low-energy configurations. The total energy of the system is the expected value of the energy function. Defining a probability transition with the Metropolis algorithm, choose configurations with probability  $e^{E(\omega)/kT}$  and weight them uniformly to find the expected value.
- (3) As a model, the physicist John Kirkwood posed the problem of whether a gas of hard disks would show a phase transitions. Consider placement of  $n$  discs of radius  $\epsilon$  in the unit square. This hard disks problems is the original motivation for the Metropolis algorithm defining a Markov chain in the configuration space.

#### Vocabulary.

- (1) Let  $X = S_n$ , the **symmetric group** of  $n$  letters, that is, the set of permutations on  $n$  letters. Let  $d(\sigma, \sigma_0)$  be a metric on the symmetric group by

$$d(\sigma, \sigma_0) = \text{minimum number of transpositions to bring } \sigma \text{ to } \sigma_0.$$

This metric is called **Cayley's distance**.

- (2) In statistical mechanics, a state of the particles is described by a **configuration**  $x$  from the **configuration space**  $\mathcal{X}$ . The configuration can be infinite or finite, continuous or discrete.

- (3) For  $\Omega$  a bounded subset  $\Lambda$  of the integer lattice in the plane, attach a value  $\pm 1$  to each site in  $\Lambda$ . This value might indicate the presence of particle there, or it might indicate an orientation (or spin) of a particle at the site. If  $\text{card}(\Lambda) = N$ , then the configuration space  $\Omega$  consists of all  $2^N$  possible assignments of values to sites in  $\Lambda$ . The physics of a configuration space  $\Omega$  is described by an energy function  $E : \Omega \rightarrow \mathbb{R}^+$ . The energy could show the total influence that neighboring particles exert on each other. This is the **Ising** model.
- (4) For a system at equilibrium, the relative frequency of a configuration  $\omega$  is given by its **Boltzmann weight**

$$e^{E(\omega)/kT}$$

where  $T$  is the temperature and  $k$  is Boltzmann's constant. For any  $\omega \in \Omega$ , its Boltzmann probability  $\text{Boltz}(\omega)$  is

$$\text{Boltz}(\omega) = \frac{e^{E(\omega)/kT}}{z}$$

where the denominator

$$z = \sum_{\omega \in \Omega} e^{E(\omega)/kT}$$

is called the **partition function**.

#### Notation.

- (1)  $\mathcal{X} = S_n$  – the **symmetric group** of  $n$  letters, that is, the group of permutations on  $n$  letters
- (2)  $\sigma, \sigma_0, \tau$  – elements of symmetric group
- (3)  $d(\sigma, \sigma_0)$  – a metric on the symmetric group
- (4)  $c(\tau)$  – number of cycles in permutation  $\tau$
- (5)  $p(\sigma)$  – probability distribution on  $S_n$
- (6)  $z$  – normalizing constant for the probability distribution,
- (7)  $\theta$  – factor defining the probability distribution
- (8)  $x$  – **configuration** from the state space, called a **configuration space**  $\mathcal{X}$  in statistical mechanics.
- (9)  $\Lambda$  – the integer lattice in the plane
- (10)  $E : \mathcal{X} \rightarrow \mathbb{R}^+$  – energy function
- (11)  $T$  – temperature and  $k$  is Boltzmann's constant.
- (12)  $\langle E \rangle$  – expected value of the energy function
- (13)  $M$  – number of samples for expected energy approximation
- (14)  $\epsilon$  – radius of small disc
- (15)  $\mathcal{X} \subset \mathbb{R}^d$  – a bounded connected open set
- (16)  $\tilde{p}(x) > 0$  – unnormalized distribution function
- (17)  $+z$  – normalization factor for  $\tilde{p}(x)$
- (18)  $\delta_x$  – Dirac delta function



### 13.9. Sources

This section is adapted from: The Markov Chain Monte Carlo Revolution by Persi Diaconis [Dia09]. The Chapter Ending Answer on random permutations is taken from the Wikipedia article Random Permutations

### 13.10. Reading Suggestion:

### 13.11. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)

### 13.12. Algorithms and Scripts

**Data:** Distribution factor  $\theta$

**Result:** Total variation distance of empirical from theoretical

**Algorithm.**

```

1 Initialize “burn-in” threshold and iterations; Initialize center  $\sigma_0$ 
2 Initialize vector to hold empirical visit count
3 Initialize  $\sigma$  as id for 1 : iterations do
4   | Generate a random transposition and apply to  $\sigma$  giving  $\sigma^*$ 
5   | If  $\sigma^*$  is closer to  $\sigma_0$  than  $\sigma$  Update  $\sigma$  as  $\sigma^*$  else
6   |   | Flip a  $\theta$ -coin
7   | end
8   | if Win then
9   |   | Update  $\sigma$  as  $\sigma^*$ 
10  | end
11  | else
12  |   | Keep current  $\sigma$ 
13  | end
14  | After “burn-in” threshold record iteration results in vector
    |   corresponding to Cayley distances in  $S_3$ .
15 end
16 Report Total variation distance of empirical from theoretical
```

#### Scripts.

**R:** library("permutations")

```

1 n <- 3 # Same as text example
2 theta <- 1/2
3 threshold <- round(3 * n * log(n)) # reasonable guess
  , based on theory
4 iterations <- threshold + 100 * factorial(n)
5 sigma0 <- id
```

```

6
7 visited <- numeric( factorial(n) )
8
9 numcycles <- function( x ) { # number of cycles,
  including length 1 cycles
10   if (is.id( x ) ) {
11     return( n )
12   } else {
13     numrealcycles <- length( get1( x ) ) # get
  element from each cycle
14     numfixed <- sum( fixed( x ) )
15     return(numrealcycles + numfixed)
16   }
17 }
18
19 cayleydist <- function(u, v) { # Cayley distance of
  perm u to perm v
20   ## u, v should be same symmetric group.
21   max( size(u), size(v) ) - numcycles( inverse(u) *
  v )
22   ## size(id) = 0, so if u = id, use size(v)
  instead
23 }
24
25 sigma <- id
26 for (i in 1:iterations) {
27   sigmastar <- rcyc(1, 2, n) * sigma # move by
  random transposition
28   if (cayleydist( sigmastar, sigma0) <= cayleydist(
  sigma, sigma0) ) {
29     sigma <- sigmastar # if closer, update sigma
30   } else {
31     if ( runif(1) <= theta ) { # toss theta-coin
32       sigma <- sigmastar      # update if win
  toss
33     }
34   }
35
36   if ( i > threshold) {
37     if ( sigma == id ) {
38       visited[1] <- visited[1] + 1
39     } else if ( sigma == as.cycle( "(12)" ) ) {
40       visited[2] <- visited[2] + 1
41     } else if ( sigma == as.cycle( "(13)" ) ) {
42       visited[3] <- visited[3] + 1
43     } else if ( sigma == as.cycle( "(23)" ) ) {
44       visited[4] <- visited[4] + 1

```

```

45     } else if ( sigma == as.cycle( "(123)" ) ) {
46         visited[5] <- visited[5] + 1
47     } else { # as.cycle( "(132)" )
48         visited[6] <- visited[6] + 1
49     }
50 }
51 }
52
53 stationary <-
54     c(1, theta, theta, theta, theta^2, theta^2)/(1 +
55       3*theta + 2*theta^2)
56 totalvariation = (1/2)* sum( abs(visited/iterations -
57   stationary) )
58 cat("Total Variation Distance of Empirical to
59   Theoretical:")
60 totalvariation)

```

### 13.13. Problems to Work for Understanding

1: Show that the transition probability matrix for the Metropolis algorithm on the symmetric group  $S_3$  is

$$\begin{array}{c}
 \begin{matrix} [123] & [213] & [321] & [132] & [231] & [312] \end{matrix} \\
 \begin{matrix} [123] \\ [213] \\ [321] \\ [132] \\ [231] \\ [312] \end{matrix}
 \begin{pmatrix}
 1-\theta & \frac{\theta}{3} & \frac{\theta}{3} & \frac{\theta}{3} & 0 & 0 \\
 \frac{1}{3} & \frac{2}{3}(1-\theta) & 0 & 0 & \frac{\theta}{3} & \frac{\theta}{3} \\
 \frac{1}{3} & 0 & \frac{2}{3}(1-\theta) & 0 & 0 & \frac{\theta}{3} \\
 \frac{1}{3} & 0 & 0 & \frac{2}{3}(1-\theta) & \frac{\theta}{3} & \frac{\theta}{3} \\
 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\
 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0
 \end{pmatrix}
 \end{array}$$

2: Choose a value of  $\theta$  ( $0 < \theta < 1$ ) and run the Markov chain on  $S_3$  for 10 iterations. How far is each row from the stationary distribution?

3: Prove that any permutation of  $n$  elements will be produced by the Knuth shuffle algorithm with probability exactly  $1/n!$ , thus yielding a uniform distribution over all such permutations.

## Markov Chain Monte Carlo

The **Markov chain Monte Carlo** (MCMC) method depends on the observation:

If  $\pi$  is the stationary distribution for an irreducible, aperiodic Markov chain, then the Markov chain can be used to sample from  $\pi$ .

To get a sample, select  $s_1 \in \mathcal{X}$  arbitrarily. For any  $n > 1$ , if  $s_{n-1} = i$ , select  $s_n = j$  with probability  $p_{ij}$ . By the Fundamental Theorem for Markov Chains and the Strong Law of Large Numbers the resulting sequence  $s_1, s_2, \dots$  has, as  $M \rightarrow \infty$ ,

$$\frac{\text{card}(\{n : n \leq M, s_n = j\})}{M} \rightarrow \pi_j$$

with probability 1.

Any large but finite part of the sequence approximates a sample from  $\pi$ . Often, one discards the first  $m$  terms of the sequence and uses the “tail” of the sequence,  $s_{m+1}, s_{m+2}, \dots, s_M$  as the sample.

Samples from  $\pi$ , however obtained, provide a way to approximate properties of  $\pi$ . Suppose  $f$  is a real-valued function on the state space  $\mathcal{X}$ . To approximate the expected value

$$\mathbb{E}[f] = \sum_{\nu=1}^N f(x_\nu) \pi_\nu$$

select a sample  $s_1, s_2, \dots, s_M$  from  $\pi$  and the ergodic theorem guarantees

$$\frac{1}{M} \sum_{\nu=1}^M f(s_\nu) \rightarrow \mathbb{E}[f]$$

as  $M \rightarrow \infty$  with convergence rate  $O(M^{-1/2})$ .

Given a reasonably sized transition probability matrix for an irreducible, aperiodic Markov chain, it is a standard exercise to find its stationary distribution. The heart of the MCMC method is the inverse problem:

Given a distribution  $\pi$  on a finite state space, find an irreducible, aperiodic Markov chain stationary on  $\pi$ .

Two solutions to this inverse problem are the Metropolis algorithm and the Metropolis-Hastings algorithm. The Metropolis algorithm was motivated by the desire to understand properties of the *Boltzmann distribution* from statistical mechanics, the branch of physics concerned with the average behavior of large systems of interacting particles.

Mathematicians Only: prolonged scenes of intense rigor.

### 14.1. Chapter Starter Question

In statistical mechanics from physics, what is the Boltzmann distribution and what does it represent?

### 14.2. A Motivational Example from Statistical Mechanics

Consider a very large but conceptually finite state space  $\mathcal{X}$ , also called a configuration space  $\mathcal{X}$ , an energy function  $E(\cdot)$  on  $\mathcal{X}$  and a fixed temperature  $T$ . Let  $\tilde{\mathcal{X}}$  be any sample of configurations selected *with replacement* from  $\mathcal{X}$ . It is desirable to let  $\tilde{\mathcal{X}}$  be larger than  $\mathcal{X}$ . The goal is to change  $\tilde{\mathcal{X}}$  so that it becomes approximately a sample from the Boltzmann distribution. Suppose  $\text{card}(\tilde{\mathcal{X}}) = \tilde{N}$  and let  $N_x$  denote the number of occurrences of  $x$  in  $\tilde{\mathcal{X}}$ . To say the sample approximates the Boltzmann distribution means

$$\frac{N_x}{\tilde{N}} = \frac{e^{-E(x)/kT}}{z}$$

for the proportionality or normalizing constant  $z$ . The denominator

$$z = \sum_{x' \in \mathcal{X}} e^{-E(x')/kT}$$

is called the partition function. In any realistic setting, the partition function is intractable, usually due to the size of  $\mathcal{X}$ . However, for any two configurations  $x$  and  $x'$

$$(14.1) \quad \frac{N_{x'}}{N_x} = \frac{e^{-E(x')/kT}}{e^{-E(x)/kT}} = e^{-(E(x')-E(x))/kT} = e^{-\Delta E/kT}.$$

This ratio does not depend on the partition function.

Now start from an irreducible, aperiodic Markov chain on  $\mathcal{X}$  with the transition probability  $P_{x,x'}$  from configuration  $x$  to  $x'$ . Also, let the transition probability matrix be symmetric,  $P_{x,x'} = P_{x',x}$  so the proposed Markov chain is reversible. Allow transitions from configurations with high energy  $E(x')$  to lower energy  $E(x)$  when they are proposed. Any downhill transition is allowed, the choice is based on convenience and naturalness. The number of times this occurs is  $P_{x',x}N_{x'}$ .

To reach equilibrium with a complete distribution of energies, not just the low energies achieved by flowing downhill, occasionally allow uphill transitions from configurations with low energy  $E(x)$  to high energy  $E(x')$  with some probability  $\mathbb{P}[x \rightarrow x']$ . The number of times the uphill transition occurs is  $P_{x,x'}N_x\mathbb{P}[x \rightarrow x']$ .

Since the Markov chain is reversible, the transition probability is symmetric and  $P_{x',x} = P_{x,x'}$ . The net flux from configurations with high energy  $E(x')$  to low energy  $E(x)$  is

$$(14.2) \quad P_{x',x}N_{x'} - P_{x,x'}N_x\mathbb{P}[x \rightarrow x'] = P_{x,x'}(N_{x'} - N_x\mathbb{P}[x \rightarrow x']).$$

In equilibrium, so that the distribution of energies in  $\tilde{\mathcal{X}}$  reflects the Boltzmann distribution very well, the net energy flux should be zero. Using equations (14.1) and (14.2) implies that the uphill probability must be

$$\mathbb{P}[x \rightarrow x'] = \frac{N_{x'}}{N_x} = e^{-\Delta E/kT}.$$

This modified Markov chain process will drive an arbitrary distribution of energies toward the Boltzmann distribution for the following reasons. Suppose the distribution has too many configurations with high energy  $E(x')$  compared with configurations with the low energy  $E(x)$ , that is,

$$\frac{N_{x'}}{N_x} > e^{-\Delta E/kT}.$$

In this case, the net flux in equation 14.2 is positive and there will be more transitions from configurations with high energy to those with low energy than in the other direction. The distribution of energies in  $\tilde{\mathcal{X}}$  will move properly towards the Boltzmann distribution. Repeating the process will produce a set of configurations whose distribution of energies approximates the Boltzmann distribution. Understanding the rate of convergence is left for further investigation.

The following is a formal statement of the Metropolis algorithm for a suitable proposed transition. For an arbitrary  $x \in \mathcal{X}$  define the Metropolis algorithm transition to a configuration  $x^*$  by the following

- (1) Define a symmetric transition probability matrix,  $P_{x,x'} = P_{x',x}$ .
- (2) Select  $y$  according to the proposed transition probability matrix.
- (3) If  $E(y) \leq E(x)$  or equivalently  $\text{Boltz}(y) \geq \text{Boltz}(x)$ , let  $x^* = y$ . In other words, always move to a lower or equal energy (equivalently, a greater or equal probability) configuration.
- (4) If  $E(y) > E(x)$  or equivalently  $\text{Boltz}(y) < \text{Boltz}(x)$ , let  $x^* = y$  with probability

$$\frac{\text{Boltz}(y)}{\text{Boltz}(x)} = e^{-\Delta E/kT}.$$

In other words, move to a higher energy (lesser probability) configuration with probability  $e^{-\Delta E/kT}$ .

- (5) Otherwise,  $x^* = x$ .

This process defines an irreducible, aperiodic Markov chain on the configuration space  $\mathcal{X}$ . The ratio is crucial to the computational utility of the Metropolis algorithm because it avoids the intractable partition function. The steps of the chain are easily computable, or at least as easy as the proposal transition. In many settings,  $\Delta E = E(x') - E(x)$  is simple to compute, often it is independent of  $\text{card}(\mathcal{X})$ . The Markov chain defined by the Metropolis algorithm can be implemented without knowing the entire transition matrix.

### 14.3. Abstraction of the Metropolis Algorithm

The Metropolis algorithm creates an easily computed Markov chain that is stationary on the desired distribution  $\pi$ . The algorithm requires only the relative weights of the limiting distribution, not the probabilities, thereby avoiding the possibly intractable normalizing constant  $z$ .

Let  $\mathcal{X}$  be a potentially large but finite state space and  $\pi(x)$  a probability mass vector on  $\mathcal{X}$ , perhaps specified only up to an unknown normalizing constant. Let  $P$  be a transition probability matrix on  $\mathcal{X}$  with  $P(x, x') > 0$  if and only if  $P(x', x) > 0$ . This is a weaker requirement than reversibility. Using parentheses instead of integer subscripts to index entries is a slight change of notation for matrices. The analogy to the previous example from statistical mechanics, along with a connection to spectral theory used later, motivates the change in notation. At the start  $P$  is unrelated to  $\pi$ . The **Metropolis algorithm** changes  $P$  to a new transition probability matrix  $Q(x, x')$  with stationary distribution  $\pi$ . Define the *acceptance ratio* as

$$A(x, x') = \frac{\pi(x')P(x', x)}{\pi(x)P(x, x')}.$$

The potential lack of a normalizing constant for the distribution  $\pi$  does not matter since it cancels in the acceptance ratio. The acceptance is the ratio of probabilities at equilibrium of moving between  $x$  and  $x'$ . If  $A(x, x') \geq 1$ , the probability at equilibrium of moving from  $x'$  to  $x$  is greater (or equal) probability than probability at equilibrium of moving from  $x$  to  $x'$ , so accept the change from  $x$  to  $x'$ . That is, accept a change to a place of greater probability. If  $A(x, x') < 1$ , the probability at equilibrium of moving from  $x'$  to  $x$  is the lesser probability, so only accept that change with some probability, see the next paragraph for the precise amount. That is, occasionally accept a change to a place of lesser probability.

The Metropolis algorithm changes  $P$  to

$$Q(x, x') = \begin{cases} P(x, x') & x \neq x', A(x, x') \geq 1 \\ P(x, x')A(x, x') & x \neq x', A(x, x') < 1 \\ P(x, x') + \sum_{z: A(x, z) < 1} P(x, z)(1 - A(x, z)) & x = x'. \end{cases}$$

The Metropolis algorithm has a simple interpretation: from  $x$ , choose  $x'$  with probability  $P(x, x')$  from the original Markov chain. Then if the acceptance ratio  $A(x, x') \geq 1$ , move to  $x'$ ; if the acceptance ratio  $A(x, x') < 1$ , flip a coin with success probability  $A(x, x')$  and move to  $x'$  if success occurs; in other cases stay at  $x$ .

The new chain satisfies

$$\pi(x)Q(x, x') = \pi(x')Q(x', x)$$

(see the exercise) and thus

$$\sum_{x \in \mathcal{X}} \pi(x)Q(x, x') = \sum_{x \in \mathcal{X}} \pi(x')Q(x', x) = \pi(x') \sum_{x \in \mathcal{X}} Q(x', x) = \pi(x').$$

Therefore,  $\pi$  is a left eigenvector with eigenvalue 1. If the Markov chain is connected, then the Fundamental Theorem of Markov Chains is in effect. After many steps

of the chain, it should have converged to a stationary distribution. That is, the chance of being at  $x$  is approximately  $\pi(x)$ , no matter what the starting state.

#### 14.4. Metropolis-Hastings Algorithm

In a 1970 paper, the statistician W. K. Hastings cast the Metropolis algorithm as a general purpose sampling algorithm, distilling the Metropolis algorithm to mathematical essentials. The following is Hastings's generalization of the Metropolis algorithm, known as the **Metropolis-Hastings algorithm**. Given a distribution  $\pi$  to sample, select any transition probability matrix  $P = (p_{ij})$  on the state space. Here the notation for matrix entries reverts again to subscripts since the application is typically for matrices on finite dimensional spaces. Unlike the Metropolis algorithm,  $P$  does not need the symmetric positivity requirement. Define the transition probability matrix  $Q = (q_{ij})$  by

$$Q_{ij} = \begin{cases} p_{ij}\alpha_{ij} & \text{if } i \neq j \\ 1 - \sum_{\nu \neq i} p_{i\nu}\alpha_{i\nu} & \text{if } i = j \end{cases}$$

where  $\alpha_{ij}$  is given by

$$\alpha_{ij} = \frac{s_{ij}}{1 + \frac{\pi_i p_{ij}}{\pi_j p_{ji}}}.$$

The values  $s_{ij}$  can be quite general so long as  $s_{ij} = s_{ji}$  for all  $i$  and  $j$  and  $0 \leq \alpha_{ij} \leq 1$ . With this choice of  $s_{ij}$  it is easy to verify that  $\pi$  is the unique stationary distribution for  $Q$ . For a symmetric  $P$ , a simple choice of  $s_{ij}$  recovers the original Metropolis algorithm.

For a given distribution  $\pi$ , different choices of  $s_{ij}$  give different Metropolis-Hastings algorithms, all of which result in a Markov chain with stationary distribution on  $\pi$ . P. H. Peskun showed that among all choices of the  $s_{ij}$ , the variance of the estimate

$$\frac{1}{M} \sum_{\nu=1}^M f(s_\nu) \rightarrow \mathbb{E}[f]$$

is asymptotically minimal for the choice that leads to the Metropolis algorithm.

#### 14.5. Convergence

A basic problem of Markov chain theory but especially for Markov chain Monte Carlo theory is: What is the rate of convergence in  $P^n(x, y) \rightarrow \pi(x)$ ? How long must the chain run to be suitably close to  $\pi$ ? It is customary to measure distance between probabilities by the total variation distance

$$\|P_x^n - \pi\|_{TV} = \frac{1}{2} \sum_y |P_x^n - \pi| = \max_{A \subset \mathcal{X}} |P^n(x, A) - \pi(A)|.$$

Probability distributions  $P_x^n$  and  $\pi$  are far apart in total variation distance if there is a “bad event”  $A$  such that  $P_x^n$  and  $\pi$  measure  $A$  differently. The goal is to show that for large  $n$  the Markov chain and the stationary distribution do not share a “bad event”. This yields the problem: Given  $P$ ,  $\pi$ ,  $x$ ,  $\epsilon > 0$ , how large must  $n$  be so that  $\|P_x^n - \pi\|_{TV} < \epsilon$ ? This question has a precise answer for only a few problems, see for example the chapter on Card Shuffling.



Suppose the Markov chain is reversible, so  $\pi(x)P(x, y) = \pi(y)P(y, x)$ . In words, reversibility means that at equilibrium the probability of going from state  $x$  to state  $y$  is the same as going from  $y$  to  $x$ . Here again the notation uses parentheses for matrix and vector entries instead of subscripts. The parenthesis notation emphasizes the following connection to  $L^2$  theory. Let the space be  $L^2(\pi)$ , the set of mappings  $\{\mathbf{g} : \mathcal{X} \rightarrow \mathbb{R}\}$  with inner product  $\langle \mathbf{g}, \mathbf{h} \rangle = \sum_x g(x)h(x)\pi(x)$ . Take  $P$  to operate on  $L^2$  by usual matrix multiplication  $P\mathbf{g}(x) = \sum_y P(x, y)g(y)$ . The property of reversibility implies  $\langle P\mathbf{g}, \mathbf{h} \rangle = \langle \mathbf{g}, P\mathbf{h} \rangle$ , so  $P$  is self-adjoint, see the exercises. The Spectral Theorem says the space has an orthonormal basis (with respect to the inner product) of right (or column) eigenvectors  $\psi_i$  and real eigenvalues  $\lambda_i$ , so  $P\psi_i = \lambda_i\psi_i$  for  $1 \leq i \leq \text{card}(\mathcal{X})$  ordered by  $1 = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{\text{card}(\mathcal{X})} \geq -1$ . Here subscripts are indexing the sets of eigenvectors and eigenvalues, not entries of vectors or matrices. Each row of  $P$  sums to 1, so  $\mathbf{1} = (1, 1, \dots, 1)^T$  is a right eigenvector corresponding to eigenvalue 1. Additionally, with respect to the weighted inner product  $\|\mathbf{1}\|^2 = \langle \mathbf{1}, \mathbf{1} \rangle = \sum_x 1 \cdot 1 \cdot \pi(x) = 1$ , so without loss of generality use  $\lambda_1 = 1$  and  $\psi_1 = \mathbf{1}$  in the convergence estimate below.

By standard inner product space manipulations (see the exercises)

$$P(x, y) = \pi(y) \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu \psi_\nu(x) \psi_\nu(y),$$

$$P^n(x, y) = \pi(y) \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu^n \psi_\nu(x) \psi_\nu(y).$$

Using the total variation metric definition and the Cauchy-Schwartz inequality

$$\begin{aligned} 2\|P_x^n - \pi\|_{TV} &= \sum_y |P^n(x, y) - \pi(y)| \\ &= \sum_y |P^n(x, y) - \pi(y)| \cdot \frac{\sqrt{\pi(y)}}{\sqrt{\pi(y)}} \\ &\leq \sqrt{\sum_y \frac{|P^n(x, y) - \pi(y)|^2}{(\sqrt{\pi(y)})^2}} \cdot \sqrt{\sum_y (\sqrt{\pi(y)})^2} \\ &= \sqrt{\sum_y \frac{|P^n(x, y) - \pi(y)|^2}{\pi(y)}}. \end{aligned}$$

Then

$$\begin{aligned}
4\|P_x^n - \pi\|_{\text{TV}}^2 &\leq \sum_y \frac{(P^n(x, y) - \pi(y))^2}{\pi(y)} \\
&= \sum_y \frac{\left(\pi(y) \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu^n \psi_\nu(x) \psi_\nu(y) - \pi(y)\right)^2}{\pi(y)} \\
&= \sum_y \pi(y) \left( \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu^n \psi_\nu(x) \psi_\nu(y) - 1 \right)^2.
\end{aligned}$$

Expand the squared term, distribute the  $\pi(y)$  terms and interchange the order of summation, factoring out terms not depending on  $y$ .

$$\begin{aligned}
&= \sum_y \pi(y) \left( \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu^{2n} \psi_\nu(x)^2 \psi_\nu(y)^2 + 2 \sum_{\nu=1}^{\text{card}(\mathcal{X})} \sum_{\mu=\nu+1}^{\text{card}(\mathcal{X})} \lambda_\nu \lambda_\mu \psi_\nu(x) \psi_\nu(y) \psi_\mu(x) \psi_\mu(y) \right. \\
&\quad \left. - 2 \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu \psi_\nu(x) \psi_\nu(y) + 1 \right) \\
&= \sum_y \left( \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu^{2n} \psi_\nu(x)^2 \psi_\nu(y)^2 \pi(y) + 2 \sum_{\nu=1}^{\text{card}(\mathcal{X})} \sum_{\mu=\nu+1}^{\text{card}(\mathcal{X})} \lambda_\nu \lambda_\mu \psi_\nu(x) \psi_\mu(y) \psi_\mu(x) \psi_\mu(y) \pi(y) \right. \\
&\quad \left. - 2 \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu \psi_\nu(x) \psi_\nu(y) \pi(y) + \pi(y) \right) \\
&= \sum_{\nu=1}^{\text{card}(\mathcal{X})} \lambda_\nu^{2n} \psi_\nu(x)^2 \sum_y \psi_\nu(y)^2 \pi(y) \\
&\quad + 2 \sum_{\nu=1}^{\text{card}(\mathcal{X})} \sum_{\mu=\nu+1}^{\text{card}(\mathcal{X})} \lambda_\nu \lambda_\mu \psi_\nu(x) \psi_\mu(x) \sum_y \psi_\nu(y) \psi_\mu(y) \pi(y) \\
&\quad - 2 \sum_{i=1}^{\text{card}(\mathcal{X})} \lambda_i \psi_i(x) \sum_y \psi_i(y) \pi(y) + \sum_y \pi(y)
\end{aligned}$$

By orthonormality,  $\sum_y \psi_\nu(y)^2 \pi(y) = \langle \psi_\nu, \psi_\nu \rangle = 1$  for  $\nu = 1, \dots, \text{card}(\mathcal{X})$ . By orthogonality,  $\sum_y \psi_\nu(y) \psi_\mu(y) \pi(y) = \langle \psi_\nu, \psi_\mu \rangle = 0$  for  $\nu = 1, \dots, \text{card}(\mathcal{X})$  and  $\mu = \nu + 1, \dots, \text{card}(\mathcal{X})$ . Recalling  $\lambda_1 = 1$  and  $\psi_1 = \mathbf{1}$ , by orthogonality  $\sum_y \psi_i(y) \pi(y) = \sum_y 1 \cdot \psi_i(y) \pi(y) = \langle \psi_1, \psi_i \rangle = 0$  for  $i = 2, \dots, \text{card}(\mathcal{X})$  while  $\sum_y \psi_1(y) \pi(y) = 1$ .

Also,  $\sum_y \pi(y) = 1$ . This leaves

$$\begin{aligned}
 &= \lambda_1^{2n} \psi_1(x)^2 + \sum_{i=2}^{\text{card}(\mathcal{X})} \lambda_i^{2n} \psi_i(x)^2 - 2\lambda_1^n \psi_1(x) + \sum_y \pi(y) \\
 &= 1 + \sum_{i=2}^{\text{card}(\mathcal{X})} \lambda_i^{2n} \psi_i(x)^2 - 2 + 1 \\
 &= \sum_{i=2}^{\text{card}(\mathcal{X})} \lambda_i^{2n} \psi_i(x)^2.
 \end{aligned}$$

Summarizing

$$(14.3) \quad \|P_x^n - \pi\|_{\text{TV}}^2 \leq \frac{1}{4} \sum_{i=2}^{\text{card}(\mathcal{X})} \lambda_i^{2n} \psi_i(x)^2.$$

This bound is the basic eigenvalue bound used to get rates of convergence for the Markov chain Monte Carlo method. Recalling Theorem 11 from Stationary Distributions, there exist constants  $\alpha \in (0, 1)$  and  $C > 0$  such that

$$\max_{x \in \mathcal{X}} \|(P^n)_i - \pi\|_{\text{TV}} \leq C\alpha^n.$$

The results here give more information, but to get good bounds on the right hand side requires knowledge of both eigenvalues and eigenvectors.

## 14.6. The Weather Example

Recall the magical land of Oz where the weather follows a pattern. If it is raining today (R), then tomorrow has a 50% chance of raining again, and a 25% chance of either having a nice day (N) or a snowy day (S) tomorrow. Similarly if it is snowing, the weather has a 50% chance of again having snow, and a 25% chance of either having a nice day, or a rainy day. Also the land of Oz never has two nice days in a row, and equally has rain or snow the day after a nice day. Further recall that for  $P^n$ , for large values of  $n$ , the row vectors approach the stationary distribution  $\pi = (2/5, 1/5, 2/5)$  in the order  $(R, N, S)$ .

Take this distribution as the desired distribution  $\pi$ . To illustrate the Markov chain Monte Carlo method, use the Metropolis-Hastings algorithm. For simplicity and in the absence of any other reasonable transition probability matrix, take the initial transition probability matrix to be uniform on the state space of weather days,  $P = (p_{ij})$  with  $p_{ij} \equiv \frac{1}{3}$ . Then  $\alpha_{ij}$  is given by

$$\alpha_{ij} = \frac{s_{ij}}{1 + \frac{\pi_i p_{ij}}{\pi_j p_{ji}}}$$

with  $s_{ij} \equiv 1$  again for simplicity and the lack of any other reasonable choice. With these choices,

$$\alpha = \begin{pmatrix} \frac{1}{2} & \frac{1}{3} & \frac{1}{2} \\ \frac{2}{3} & \frac{1}{2} & \frac{2}{3} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{2} \end{pmatrix}.$$

Following the construction of the Metropolis-Hastings algorithm

$$Q = \begin{pmatrix} \frac{13}{18} & \frac{1}{9} & \frac{1}{6} \\ \frac{2}{9} & \frac{1}{9} & \frac{2}{9} \\ \frac{1}{6} & \frac{1}{9} & \frac{13}{18} \end{pmatrix}.$$

Then  $\pi = (2/5, 1/5, 2/5)$  is a stationary distribution of  $Q$ , just as it is for  $P$ . Comparing the rates of convergence is interesting too. The eigenvalues of  $P$  are  $1, 1/4, -1/4$ , so the rate of convergence of  $P^n$  is about like  $(1/4)^n$ . On the other hand, the eigenvalues of  $Q$  are  $1, 5/9, 4/9$ , so the rate of convergence of  $Q^n$  is about like  $(5/9)^n$ , much slower. This is not surprising, since sampling the stationary distribution with the Metropolis algorithm is not as direct.

The Markov chain with  $Q$  as transition probability matrix is reversible. After 5 steps the square of the total variation distance of the distribution from state 1, Rain, from the stationary distribution is approximately  $7.95 \times 10^{-4}$  while the bound from (14.3) is  $8.94 \times 10^{-4}$ . After 10 steps the square of the total variation distance of the distribution from state 1 from the stationary distribution is approximately  $2.05 \times 10^{-6}$  while the bound from (14.3) is  $2.45 \times 10^{-6}$ . Regression analysis gives

$$\|(Q^n)_{1,\cdot} - \pi\|_{TV} \approx 0.5295 \cdot (0.5538)^n,$$

about what is expected.

## 14.7. Example with Continuous State Space

Consider three particles each randomly located in the square  $[0, 1]^2 \subset \mathbb{R}^2$  with positions  $(x_{i1}, x_{i2})$  for  $i = 1, 2, 3$ . The state space is  $\mathcal{X} = [0, 1]^6$ . Suppose the positions of the particles are distributed according to the density

$$\pi(x) = \pi(x_1, x_2, x_3) = \frac{1}{z} \exp \left[ -C \sum_{i=1}^3 \|x_i\| - D \sum_{i < j} \frac{1}{\|x_i - x_j\|} \right]$$

where  $\|\cdot\|$  is the usual Euclidean norm on  $\mathbb{R}^2$ ,  $C$  and  $D$  are fixed positive constants and  $z$  is the normalizing constant or partition function. In this density the first sum pushes the particle towards the origin, the second sum pushes them away from each other.

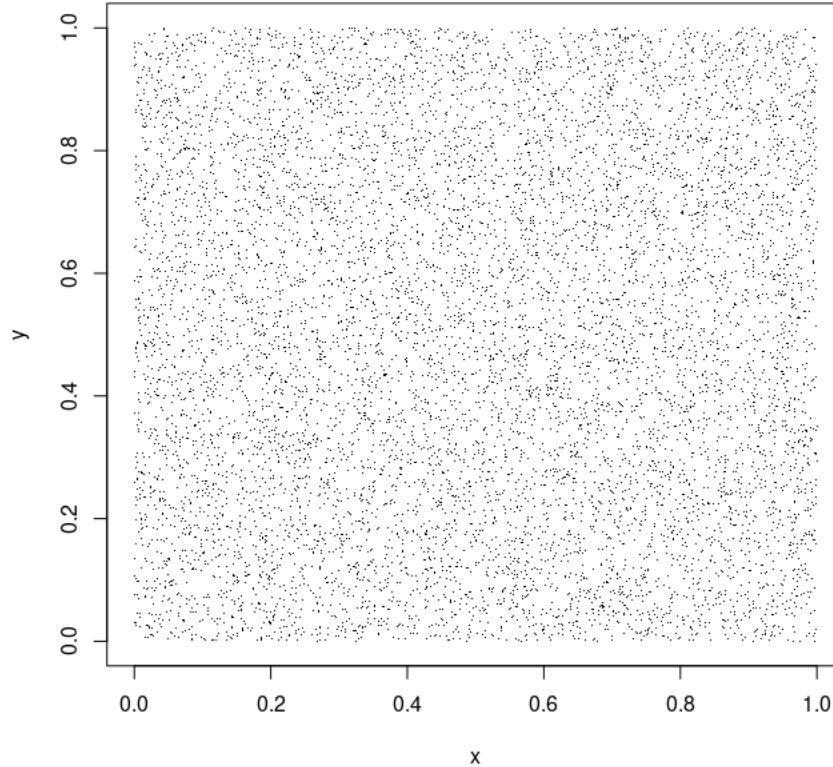
To create a Markov chain with  $\pi$  as its stationary distribution, use the Metropolis algorithm. Given  $X_n$ , first choose  $y \in [0, 1]^6$  from the uniform distribution on  $\mathcal{X}$ . Then with probability  $r = \min[1, \pi(y)/\pi(x)]$ , accept  $X_{n+1} = y$ , otherwise reject  $y$  and  $X_{n+1} = x$ . Then this Markov chain has  $\pi$  as its stationary distribution. The later section on Convergence to the Stationary Distribution will show that with  $C = D = \frac{1}{10}$  the rate of convergence is

$$\|\text{dist}(X_n) - \pi\|_{TV} \leq (0.883)^n$$

so that after 38 steps, the total variation distance between the Markov chain and the stationary distribution is less than 0.01.

A plot of the stationary distribution is Figure 14.1.

**Figure 14.1.** Plot of points  $x_1, x_2, x_3$  from step 100 to step 3000 in the Metropolis algorithm simulation of the stationary distribution  $\pi$  for the continuous state space Markov chain.



#### 14.8. Example with Unbounded Continuous State Space

Let the state space be  $\mathcal{X} = \mathbb{R}$  with target density the double exponential or Laplace distribution.  $\pi(x) = e^{-|x|}/2$ . It is easy to simulate the double exponential density using the standard technique of choosing a uniform random deviate and then applying the inverse of the cumulative distribution function, so this is an illustrative example rather than a practical simulation method for the double exponential distribution.

Use another version of the Metropolis algorithm. Choose the initial state  $x_0$  uniformly at random from the interval  $[-2, +2]$ . At succeeding steps, first propose to move from state  $x$  to  $y$  chosen uniformly at random from the interval  $[x-2, x+2]$ . With probability  $\min[1, \pi(y)/\pi(x)]$ , accept the proposal  $y$  which becomes the new state, otherwise reject it and remain at  $x$ . Again, this procedure creates a Markov chain with  $\pi$  as its stationary distribution.

The later section on Convergence to the Stationary Distribution will show that a theoretical upper bound on the rate of convergence is

$$\|\text{dist}(X_n) - \pi\|_{TV} \leq (0.983)^{1+n/439.56} + (2 \cdot (20.04)^{n/439.56})(0.993)^n$$

so that after 120,000 steps, the total variation distance between the Markov chain and the stationary distribution is less than 0.01. The R script in the Algorithms section shows that after about 48,000 steps total variation distance between this Markov chain and the stationary distribution is less than 0.05. Either way, the convergence to a stationary distribution is much slower than other examples.

### 14.9. Chapter Ending Answer

In statistical mechanics and mathematics, a Boltzmann distribution is a probability distribution or probability measure that gives the probability that a system will be in a certain state or “configuration” as a function of that state’s energy and the temperature of the system. The distribution is expressed in the form:

$$p_i \propto e^{-\frac{\varepsilon_i}{kT}}$$

where  $p_i$  is the probability of the system being in state  $i$ ,  $\varepsilon_i$  is the energy of that state, and a constant  $kT$  of the distribution is the product of Boltzmann’s constant  $k$  and thermodynamic temperature  $T$ . With this distribution, states with lower energy have a higher probability of being occupied.

### 14.10. Chapter Summary

#### Key Concepts.

- (1) With Markov chain Monte Carlo, to get a sample, select  $s_1 \in \mathcal{X}$  arbitrarily. If  $s_{k-1} = i$ , select  $s_k = j$  with probability  $p_{ij}$ . By the Fundamental Theorem for Markov Chains and the Strong Law of Large Numbers for any  $k > 1$ , the resulting sequence  $s_1, s_2, \dots$  has, as  $M \rightarrow \infty$ ,

$$\frac{\text{card}(\{k : k \leq M, s_k = j\})}{M} \rightarrow \pi_j$$

with probability 1.

- (2) The heart of the MCMC method is the inverse problem: Given a distribution  $\pi$  on a finite state space, find an irreducible, aperiodic Markov chain that is stationary on  $\pi$ . The solution to this inverse problem is the **Metropolis algorithm**.
- (3) The formal statement of the Metropolis algorithm for a suitable proposed transition is: For an arbitrary  $x \in \mathcal{X}$  define the transition to a configuration  $x^*$ .
  - (a) Select  $x'$  according to the proposed transition.
  - (b) If  $E(x') \leq E(x)$  or equivalently  $\text{Boltz}(x') \geq \text{Boltz}(x)$ , let  $x^* = x'$ . In other words, always move to a lower energy (higher probability) configuration.

- (c) If  $E(x') > E(x)$  or equivalently  $\text{Boltz}(x') < \text{Boltz}(x)$ , let  $x^* = x'$  with probability

$$\frac{\text{Boltz}(x')}{\text{Boltz}(x)} = e^{-\Delta E/kT}.$$

- (d) Otherwise,  $x^* = x'$ .

- (4) For the Metropolis-Hastings algorithm, given a distribution  $\pi$  to sample, select any transition probability matrix  $P = (p_{ij})$  on the state space. Unlike the Metropolis algorithm,  $P$  does not need to be symmetric. Define the transition probability matrix  $Q = (q_{ij})$  by

$$Q_{ij} = \begin{cases} p_{ij}\alpha_{ij} & \text{if } i \neq j \\ 1 - \sum_{k \neq i} q_{ik} & \text{if } i = j \end{cases}$$

where  $\alpha_{ij}$  is given by

$$\alpha_{ij} = \frac{s_{ij}}{1 + \frac{\pi_i p_{ij}}{\pi_j p_{ji}}}.$$

The values  $s_{ij}$  can be quite general so long as  $s_{ij} = s_{ji}$  for all  $i$  and  $j$  and  $0 \leq \alpha_{ij} \leq 1$ .

#### Vocabulary.

- (1) The **Markov chain Monte Carlo** (MCMC) method depends on the observation that if  $\pi$  is the stationary distribution for an irreducible, aperiodic Markov chain, then the Markov chain can be used to sample from  $\pi$ .
- (2) The heart of the MCMC method is the inverse problem: Given a distribution  $\pi$  on a finite state space, find an irreducible, aperiodic Markov chain that is stationary on  $\pi$ . Two solutions to this inverse problem are the **Metropolis algorithm** and the **Metropolis-Hastings algorithm**.
- (3) In a 1970 paper, the statistician W. K. Hastings cast the Metropolis algorithm as a general purpose sampling algorithm, distilling the Metropolis algorithm to mathematical essentials. Hastings's generalization of the Metropolis algorithm is the **Metropolis-Hastings algorithm**.
- (4) Suppose the Markov chain is reversible, so  $\pi(x)P(x, y) = \pi(y)P(y, x)$ . In words, reversibility means that at equilibrium the probability of going from state  $x$  to state  $y$  is the same as going from  $y$  to  $x$ .

#### Notation.

- (1)  $\pi$  – the stationary distribution for an irreducible, aperiodic Markov chain
- (2)  $\mathcal{X}$  – state space for Markov chain
- (3)  $s_1$  – arbitrary element of the state space
- (4)  $n > 1$  – arbitrary step in Markov chain sample
- (5)  $s_{n-1}, s_n$  – successive steps in Markov chain sample
- (6)  $p_{ij}$  – transition probability from state  $i$  to state  $j$
- (7)  $M, m$  – large sample sizes in Markov chain sample
- (8)  $f$  – arbitrary function on the state space

- (9)  $E(\cdot)$  – energy function
- (10)  $T$  – temperature
- (11)  $\tilde{\mathcal{X}}$  be any sample of configurations selected *with replacement* from  $\mathcal{X}$
- (12)  $\text{card}(\tilde{\mathcal{X}}) = \tilde{N}$
- (13)  $N_x$  – the number of occurrences of  $x$  in  $\tilde{\mathcal{X}}$
- (14)  $z = \sum_{x' \in \mathcal{X}} e^{-E(x')/kT}$  – the partition function.
- (15)  $k$  – Boltzmann constant
- (16)  $\text{Boltz}(x')$  – Boltzmann probability density
- (17)  $P(x, x')$  – transition probability matrix on  $\mathcal{X}$
- (18)  $P = (p_{ij})$  – transition probability matrix on the state space
- (19)  $Q$  – alternative transition probability matrix from Metropolis or Metropolis Hastings algorithm
- (20)  $L^2(\pi)$  – the set of mappings  $\{\vec{g} : \mathcal{X} \rightarrow \mathbb{R}\}$  with inner product  $\langle \vec{g}, \vec{h} \rangle = \sum_x g(x)h(x)\pi(x)$
- (21)  $\beta_i$  – real eigenvalues
- (22)  $\vec{\psi}_i$  – eigenvectors
- (23)  $(x_{i1}, x_{i2})$  for  $i = 1, 2, 3$  – positions for three particles each randomly located in the square  $[0, 1]^2 \subset \mathbb{R}^2$
- (24)  $C$  and  $D$  – fixed positive constants

### 14.11. Sources

This section is adapted from: “The Evolution of Markov Chain Monte Carlo Methods” by Matthew Richey [Ric10] and “The Markov chain Monte Carlo revolution” by Persi Diaconis [Dia09]. The examples of the continuous state space and the unbounded state space is adapted from [JLL<sup>+</sup>21].

### 14.12. Reading Suggestion:

### 14.13. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)



### 14.14. Algorithms and Scripts

**Data:** Desired stationary distribution

**Result:** Approximate stationary distribution

1 *Initialization of Matrices*

2 Load Markov chain library

3 Set number of states

4 Set simple uniform transition probability matrix

5 Set state names

6 Set desired stationary distribution

**Algorithm.**

7 Set up matrix with  $s$  values

8 Set matrix with  $\alpha$  values according to algorithm

9 Set new probability transition matrix

10 Set markovchain object

11 Set length of long sample path and start position for sample

12 Slice the long sample path from the transient time to the end

13 In the slice count the appearance of each state

14 Empirical stationary distribution

**Algorithm 16:** Metropolis-Hastings algorithm

#### Scripts.

**R:** R script for metHast.R

```

1 library("markovchain")
2
3 nStates <- 3
4 P <- matrix(rep(1/nStates, nStates * nStates),
5             nrow=nStates, byrow=TRUE)
6 stateNames <- c("Rain", "Nice", "Snow")
7 rownames(P) <- stateNames
8 colnames(P) <- stateNames
9
10 pi <- c(2/5, 1/5, 2/5)
11 s <- matrix(rep(1, nStates * nStates),
12            nrow=nStates, byrow=TRUE)
13
14 alpha <- matrix(0, nStates, nStates)
15 for (i in 1:nStates) {
16   for (j in 1:nStates) {
17     alpha[i, j] <- s[i, j] * (1 / (1 + (pi[i]/pi[
18       j])*(P[i, j]/P[j, i])))
19   }
20 }
21 Q <- matrix(0, nStates, nStates)
22 for (i in 1:nStates) {

```

```

23     for (j in 1:nStates) {
24         if (i != j) {
25             Q[i, j] <- P[i, j] * alpha[i, j]
26         }
27     }
28     Q[i, i] <- 1 - sum( Q[i, ] )
29 }
30
31 hastMetWeather <- new("markovchain", states =
    stateNames,
32                         transitionMatrix = Q,
33                         name = "hastMetWeather")
34 cat( "Steady State Distribution: ", steadyStates(
    hastMetWeather), "\n" )
35
36 start <- 900
37 end <- 1000
38 hastMetWeatherSim <- rmarkovchain(n=end, object=
    hastMetWeather,
39                                   t0="Nice")
40 cat("Simulation Results\n")
41 cat( "Rain:", sum( hastMetWeatherSim[(start+1):end]
    == "Rain")/(end-start), "\n")
42 cat( "Nice:", sum( hastMetWeatherSim[(start+1):end]
    == "Nice")/(end-start), "\n")
43 cat( "Snow:", sum( hastMetWeatherSim[(start+1):end]
    == "Snow")/(end-start), "\n")

```

### 14.15. Problems to Work for Understanding

- 1: For the Metropolis algorithm, show that

$$\pi(x)Q(x, x') = \pi(x')Q(x', x).$$

+

- 2: Consider the following Markov Chain:  $N$  black balls and  $N$  white balls are placed in two urns so that each contains  $N$  balls. At each step one ball is selected at random from each urn and the two balls interchange urns. Let  $N = 3$  and the state of the system is the number of white balls in the first urn.

- What is the probability transition matrix  $P$ ?
- What is the stationary distribution?
- What is the matrix  $\alpha$  of entries  $\alpha_{ij}$  in the Metropolis-Hastings algorithm?
- Choose a satisfactory transition matrix and then create the matrix  $Q$  in the Metropolis-Hastings algorithm.
- Find the eigenvalues of  $P$  and the approximate rate of convergence to the stationary distribution.

- (f) Find the eigenvalues of  $Q$  and the approximate rate of convergence to the stationary distribution.

3: Consider the second Ehrenfest urn model with  $N = 4$ ,  $p = q = \frac{1}{2}$  and transition probability matrix

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{8} & \frac{1}{2} & \frac{3}{8} & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\ 0 & 0 & \frac{3}{8} & \frac{1}{2} & \frac{1}{8} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

- Show that this Markov chain is irreducible, positive recurrent, aperiodic.
- Find the stationary distribution  $\pi$ .
- Show the Markov chain is reversible.
- Find the eigenvalues and corresponding eigenvectors, ordered by decreasing eigenvalue.
- Using the inner product weighted by  $\pi$ , find the normalized orthonormal eigenvector basis.
- Show that

$$P(x, y) = \pi(y) \sum_{i=1}^5 \lambda_i \psi_i(x) \psi_i(y).$$

- Using the results from the previous problem, find the upper bound (14.3) for the square of the total variation distance of the distribution starting from state 5, with all balls in the first urn, from the stationary distribution.
  - With numerical computation, check the inequality for 5 and 10 steps of the Markov chain.
- Suppose the Markov chain is reversible, so  $\pi(x)P(x, y) = \pi(y)P(y, x)$ . Let the space be  $L^2(\pi)$ , the set of mappings  $\{g : \mathcal{X} \rightarrow \mathbb{R}\}$  with inner product  $\langle \mathbf{g}, \mathbf{h} \rangle = \sum_x \mathbf{g}(x)\mathbf{h}(x)\pi(x)$ . Then  $P$  operates on  $L^2(\pi)$  by multiplication  $P\mathbf{g}(x) = \sum_y P(x, y)\mathbf{g}(y)$ . Show that the property of reversibility implies  $\langle P\mathbf{g}, \mathbf{h} \rangle = \langle \mathbf{g}, P\mathbf{h} \rangle$ , so  $P$  is self-adjoint.
- For self-adjoint matrix  $P$  and stationary distribution  $\pi$ , with an orthonormal basis (with respect to the inner product  $\langle \mathbf{g}, \mathbf{h} \rangle = \sum_x \mathbf{g}(x)\mathbf{h}(x)\pi(x)$ ) with right eigenvectors  $\psi_i$  and real eigenvalues  $\lambda_i$ , so  $P\psi_i = \lambda_i\psi_i$  for  $1 \leq i \leq \text{card}(\mathcal{X})$  ordered by  $1 = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{\text{card}(\mathcal{X})} \geq -1$ , show that

$$P(x, y) = \pi(y) \sum_{i=1}^{\text{card}(\mathcal{X})} \lambda_i \psi_i(x) \psi_i(y).$$

## The Ising Model

Magnets are common objects but magnetism itself is enigmatic. Heating a ferromagnetic material such as iron causes it to lose magnetism. Slow cooling allows the material to magnetize again. From 1922 to 1925 Wilhelm Lenz and his student Ernst Ising developed what is now called the Ising model to explain this phase transition in magnetism caused by heating or cooling. The Ising model connects electromagnetic theory with statistical mechanics. Exploring the Ising model for the magnetic phase transition uses Markov chains. The goal of this chapter is to describe applications of the Metropolis algorithm to the Ising model for magnetism.

Mathematically Mature: may contain mathematics beyond calculus with proofs.

### 15.1. Chapter Starter Question

What is a phase transition? What causes phase transitions? What are some examples of phase transitions?

### 15.2. Magnetism and the Ising Model

In a magnetic material such as iron, the atoms each have a magnetic moment. A piece of iron has small regions or “domains” that are completely magnetized because the atoms align in the same direction. The overall energy of neighboring atoms in the domain is lower when the moments are parallel. If the energy of neighboring atoms and domains were the only consideration, a magnetic material would settle into a magnetized configuration, but heat tends to randomize the magnetic moment directions. On a large scale, the directions of the domains are not aligned so average magnetization is about zero.

In the physics of magnetism, the Curie temperature  $T_c$  is the temperature above which certain materials lose their permanent magnetic properties. The Curie temperature is named after Pierre Curie, who showed that magnetism disappears above

a critical temperature. Above  $T_c$  thermal energy disrupts the tendency toward magnetic dipole alignment, and materials become just weakly magnetic.

The **Ising model** is a simple model of a ferromagnet's domain alignment due to energy and heat. The model describes the tendency for neighboring atoms to align their magnetic fields with each other or with an external magnetic field. The Ising model exhibits a **phase transition** in the magnetization, a dramatic change between differently ordered magnetic states as a parameter passes through a critical value. Moreover, the 2-dimensional Ising model is one of the most important theoretical statistical mechanical models. As with all mathematical models, the aim is to find the simplest framework that exhibits important properties of the physical system. With just the simple elements of binary variables on a regular grid, the Ising model exhibits phase transitions.

The Ising model is a lattice model of atomic magnetic dipoles aligned up or down in some fixed direction. A 1-dimensional Ising model pictures dipoles regularly spaced along a line. A 2-dimensional Ising model is a square lattice, and a 3-dimensional Ising model is a cubic lattice. Each atom interacts with its nearest neighbors. The goal of the model is to find  $T_c$ . Interestingly, the 1-dimensional Ising model does not have a phase transition, first proved by Ernst Ising in 1925. A 1944 result of Lars Onsager gives a relation for the exact value for the critical temperature in the 2-dimensional Ising model:

$$\frac{k_{\text{Boltz}} T_c}{J} = \frac{2}{\log(1 + \sqrt{2})} \approx 2.269$$

where  $k_{\text{Boltz}}$  is the Boltzmann constant from statistical mechanics and  $J$  is a proportionality constant for the energy of a dipole alignment.

For definiteness for this application of the Metropolis algorithm, assume a planar square lattice with  $N^2$  sites. An  $N \times N$  matrix represents the square lattice, the first row at the top, and the  $N$ th row at the bottom, the first column at the left, the  $N$ th column at the right. At each lattice site  $(i, j)$ , there is a *spin* represented by  $\omega_{i,j} = \pm 1$ . A configuration is a matrix of spins,  $\omega = (\omega_{1,1}, \omega_{1,2}, \dots, \omega_{N,N})$ . Define  $\Omega$  as the set of all possible configurations so  $\text{card}(\Omega) = 2^{N^2}$ . The magnetic energy (also called the Hamiltonian) of a configuration is

$$E(\omega) = -J \sum_{i,j=1}^N \sum_{k=1}^4 \omega_{i,j} \omega_{\langle i,j \rangle[k]} - H \sum_{i=1}^N \omega_i$$

where  $J > 0$  is the nearest-neighbor affinity (a proportionality constant with units of energy for the strength of the binding between neighbors),  $H \geq 0$  represents the external magnetic field and  $\langle i, j \rangle$  indicates the set of 4 sites that are periodic nearest neighbors, sites in the lattice with a horizontal or vertical bond. For the top row with  $i = 1$ , periodic means  $\langle 1, j \rangle = \{(2, j), (1, j - 1), (N, j), (1, j + 1)\}$ , interpreting periodically if  $j = 1$  or  $j = N$ . Similarly for the bottom row, and the leftmost and rightmost columns. The periodic boundary conditions mean that boundary sites are not treated differently than interior sites and make the finite grid simulate an infinite grid. For purposes of the example, assume there is no external field, so  $H = 0$  and that  $J = 1$ .

The probability distribution of spin configurations is proportional to the **Boltzmann weight**  $\text{Boltz}(\omega) = e^{-E(\omega)/(k_{\text{Boltz}}T)}$  where  $k_{\text{Boltz}}$  is the Boltzmann constant and  $T$  is the absolute temperature, so  $k_{\text{Boltz}}T$  has units of energy. The energy units are chosen to make  $k_{\text{Boltz}}T_C = \frac{2}{\log(1+\sqrt{2})}$ . This section uses the combination  $k_{\text{Boltz}}T$  consistently for the heat energy at temperature  $T$  to emphasize the connection with statistical mechanics, with  $0 \leq k_{\text{Boltz}}T \leq 10$  for illustration. Given a configuration, the Boltzmann weight is proportional to the probability that configuration will appear at temperature  $T$ . For completely ordered configurations with  $\omega_{i,j} \equiv +1$  or  $\omega_{i,j} \equiv -1$ ,  $E(\omega) = -J \cdot 4N^2$  (low magnetization energy) and  $\text{Boltz}(\omega) = e^{J \cdot 4N^2/(k_{\text{Boltz}}T)}$  is large (relatively higher probability). For highly disordered configurations with  $\omega_{i,j} = \pm 1$  distributed randomly,  $E(\omega) \approx 0$  (higher magnetization energy) and  $\text{Boltz}(\omega) \approx e^{-0/(k_{\text{Boltz}}T)} \approx 1$  is small (relatively lower probability).

For a configuration  $\omega$  the net spin is

$$M(\omega) = \sum_{i,j=1}^N \omega_{i,j}.$$

The **magnetization** at temperature  $T$  is  $\mathbb{E}[M]_T$  is the expected value of  $M(\omega)$  with respect to the Boltzmann weight:

$$\begin{aligned} \mathbb{E}[M]_T &= \sum_{\omega \in \Omega} M(\omega) \text{Boltz}(\omega) \\ &= \frac{1}{z} \sum_{\omega \in \Omega} M(\omega) e^{-E(\omega)/(k_{\text{Boltz}}T)}. \end{aligned}$$

Recall that the denominator

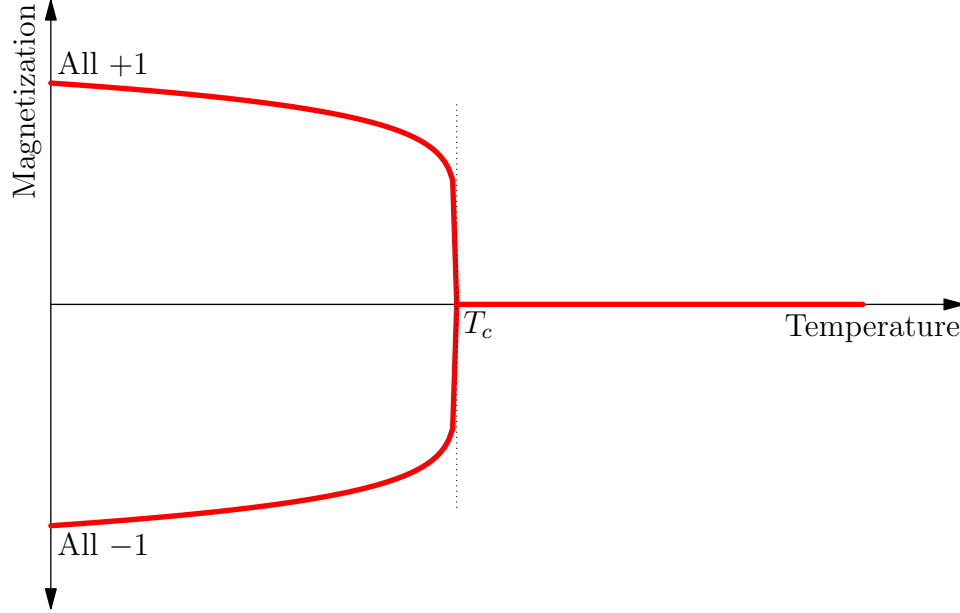
$$z = \sum_{\omega \in \Omega} e^{-E(\omega)/(k_{\text{Boltz}}T)}$$

is called the partition function.

This model exhibits some general features. At high temperatures there is no correlation between sites, states are essentially uniformly distributed and hence  $\mathbb{E}[M]_T$  is near zero. This highly disordered configuration is not magnetic. Lowering the temperature to a critical value called the Curie temperature  $T_c$ , spontaneous magnetization occurs. The model goes to one of the highly ordered state of all +1 or all -1 spins. See Figure 15.1 for a schematic diagram of the phase transition. The Curie temperature is a critical temperature below which sites influence each other at long distances. It is impractical to directly compute the expected magnetization since the number of configurations is too large. Even for  $N = 5$ , to directly compute the magnetization requires  $2^{25}$  matrices with 25 entries, over 838 million values.

### 15.3. The Metropolis Algorithm and the Ising Model

Since direct calculation is unfeasible, the goal is to apply the Metropolis algorithm to the Ising model to find  $T_c$ . To do that, run the Markov chain Monte Carlo method at different temperatures to find the average magnetization as a function of temperature to find where the phase change occurs. Figure 15.2 and Figure 15.3



**Figure 15.1.** Schematic magnetic phase diagram for the Ising model.

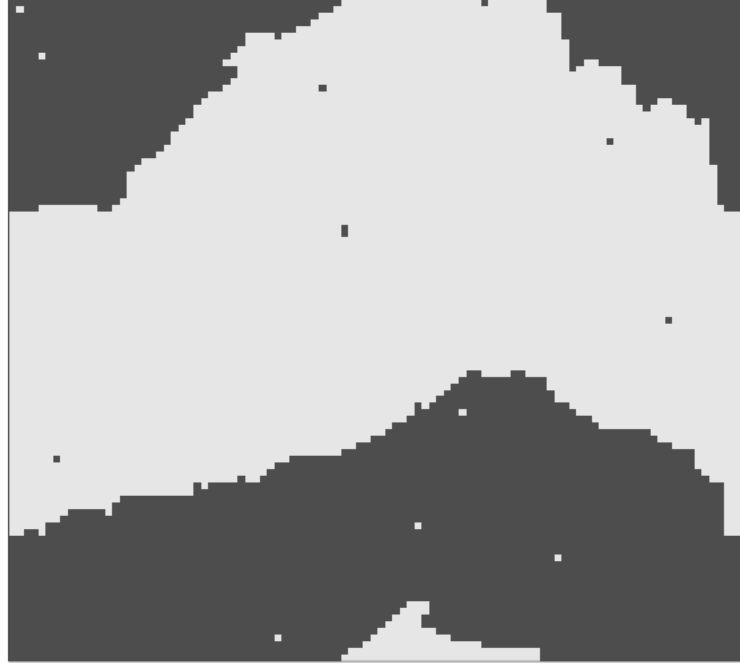
are snapshots of applying the Metropolis algorithm to the Ising model. Figure 15.2 shows large areas of consistent magnetization after 500,000 Markov chain steps started from a random configuration at a normalized temperature  $2.2 < T_c$ . Figure 15.2 appears random even after 50,000,000 Markov chain steps started from a random configuration at a temperature  $5.0 > T_c$ .

The key idea behind the algorithm is to emphasize the low energy subset of configurations and discount the rest. The Metropolis algorithm takes a random walk through the configuration space, visiting more frequently occurring spin configurations more often. In the words of the original Metropolis algorithm paper: “Instead of choosing configurations randomly, then weighting them with  $e^{-E/(k_{\text{Boltz}}T)}$ , instead choose configurations with probability  $e^{-E/(k_{\text{Boltz}}T)}$  and weight them evenly”. The Metropolis algorithm for the Ising model proceeds as follows:

- (1) Visit all lattice sites  $(i, j)$  in some deterministic order. For example, visit across the first row, then across the second row, and so on to the last row.
- (2) As each site is visited, calculate the change in energy that would result from flipping the spin at the selected site. If  $\omega$  is the visited configuration and  $\omega'$  is the configuration with the flipped spin at the visited site, then

$$\Delta E = E(\omega') - E(\omega) = -2J(\omega'_{(i,j)} - \omega_{(i,j)}) \sum_{k=1}^4 \omega_{\langle i,j \rangle[k]}$$

where the sum is only over the four nearest neighbors of the  $(i, j)$  site. The computational cost of updating a site is both small and independent of the size of the lattice.



**Figure 15.2.** A  $100 \times 100$  Ising model at  $T = 2.2$  after 500,000 steps.

- (3) The acceptance rule is: if energy increases,  $E(\omega') > E(\omega)$  or equivalently  $\text{Boltz}(\omega') < \text{Boltz}(\omega)$ , let  $\omega^* = \omega'$  with acceptance probability

$$\frac{\text{Boltz}(\omega')}{\text{Boltz}(\omega)} = e^{-\Delta E / k_{\text{Boltz}} T}.$$

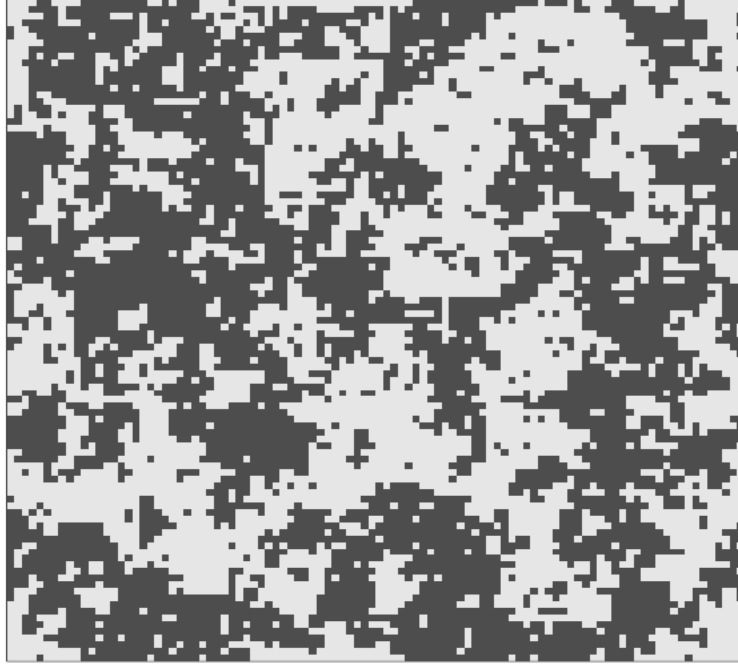
- (4) Otherwise, energy decreases, so accept the change,  $\omega^* = \omega'$ .

Verifying the Markov chain of configuration changes is irreducible and aperiodic is routine.

The alternative Glauber dynamics algorithm (or in a different context the *random chain algorithm*) is:

- (1) The visitation rule between configurations is to pick a lattice site  $(i, j)$  uniformly at random from  $i, j = 1, 2, 3, \dots, N$ .
- (2) As each site is visited, calculate the change in energy that would result from flipping the spin at the selected site. If  $\omega$  is the visited configuration and  $\omega'$





**Figure 15.3.** A  $100 \times 100$  Ising model at  $T = 5.0$  after 50,000,000 steps.

is the configuration with the flipped spin at the visited site, then

$$\Delta E = E(\omega') - E(\omega) = -2J(\omega'_{(i,j)} - \omega_{(i,j)}) \sum_{k=1}^4 \omega_{\langle i,j \rangle[k]}$$

where the sum is only over the four nearest neighbors of the  $(i, j)$  site. The computational cost of updating a site is both small and independent of the size of the lattice.

- (3) The current configuration  $\omega$  becomes the flipped site configuration  $\omega'$  with acceptance probability

$$\frac{e^{-\Delta E/k_{\text{Boltz}}T}}{1 + e^{-\Delta E/k_{\text{Boltz}}T}}.$$

- (4) Otherwise,  $\omega^* = \omega$ .

Verifying the Markov chain of configuration changes is irreducible and aperiodic is routine.

Each algorithm has advantages and disadvantages. For the Metropolis algorithm at low temperatures unfavorable flips are rare, resulting in a (nearly) deterministic flip rule along a deterministic path. This can result in the algorithm getting trapped in patterns in the lattice. On the other hand, with random sampling of sites in the Glauber algorithm, taking 10,000 steps on a  $100 \times 100$  lattice will miss about  $3,679 = 10,000/e$  sites, see the exercises. Therefore, it takes more steps than the size of the lattice to ensure visiting all sites. Also, the acceptance probability in the Glauber algorithm is less than the acceptance probability in the Metropolis algorithm, see the exercises. So the Glauber algorithm converges more slowly than the Metropolis algorithm. The survey article by Diaconis and Saloff [DSC98] presents estimates on rates of convergence indicating slow convergence for the Ising model algorithms considered here.

The two scripts below illustrate the global approach to the Ising model and the Monte Carlo Markov chain method. The script `isingDist.R` calculates the entire configuration space, the individual energy of each configuration and the partition function. However it is only practical for  $N = 2, 3, 4$ , not refined enough to demonstrate the phase transition. The second script `isingMetropolis.R` illustrates the Monte Carlo Markov chain approach. The script directly implements the Metropolis method above but is not general. For a general approach, see the R package `IsingSampler` [Eps20] and for another implementation in Python, see [Sch18].

The comprehensive and very readable survey article [Hay21] provides interactive graphics for comparing the Metropolis and Glauber algorithms directly, mixing the visitation and acceptance rules for the Metropolis and Glauber algorithms, using different visitation rules for the Metropolis algorithm, and testing the effects of different initial and boundary conditions. The article also has figures for the Boltzman weight function at various temperatures, comparison of the acceptance functions, comparisons of rates of convergence, and explanations for the growth of shapes in the graphics. Finally, the article has a well-researched history of the Metropolis and Glauber algorithms.

## 15.4. Chapter Ending Answer

A phase transition is dramatic change in state as a parameter passes through a critical value. In physical and chemical systems, the transition occurs from the addition or removal of energy, usually in the form of heat, but it can also result from pressure changes or other causes. Examples of phase transitions are the freezing of water into ice, or the reverse melting, the vaporization of water to steam or the reverse condensation. Biological systems exhibit phase transitions at the molecular, cellular, and even the organism level. In card-shuffling the rapid transition from relatively ordered to completely disordered after  $O(n \log n)$  shuffles is an example of a mathematical phase transition.

## 15.5. Chapter Summary

### Key Concepts.

- (1) The Ising model is a lattice model of spins for atoms with magnetic dipoles either up or down in some fixed direction. The Ising model exhibits a **phase**

**transition** in the magnetization, a dramatic change in state as a parameter passes through a critical value.

- (2) It is impractical to directly compute the expected magnetization since the number of configurations is too large.
- (3) Estimates on rates of convergence indicate slow convergence for the Ising model Metropolis algorithm considered here. The slow convergence is consistent with the number of steps needed to ensure visiting most sites.

#### Vocabulary.

- (1) The **Ising model** is a simple model of a ferromagnet.
- (2) A **phase transition** is a dramatic change in state as a parameter passes through a critical value.
- (3) The **Boltzmann weight**  $\text{Boltz}(\omega) = e^{-E(\omega)/(k_{\text{Boltz}}T)}$  where  $k_{\text{Boltz}}$  is the Boltzmann constant, so  $k_{\text{Boltz}}T$  has units of energy.
- (4) For a configuration  $\omega$  let

$$M(\omega) = \sum_{i,j=1}^N \omega_{i,j}.$$

- (5) The **magnetization** at temperature  $T$  is  $\mathbb{E}[M]_T$  is the expected value of  $M(\omega)$ .
- (6) **Glauber dynamics** is the algorithm that selects sites at random in the lattice and computes magnetization in a Markov chain.

#### Notation.

- (1)  $T_c$  – the temperature above which certain materials lose their permanent magnetic properties
- (2)  $k_{\text{Boltz}}$  – the Boltzmann constant from statistical mechanics
- (3)  $J$  – a proportionality constant for the energy of alignment
- (4)  $N$  – number of rows and columns in 2-dimensional lattice with  $N^2$  sites
- (5)  $(i, j)$  – lattice site
- (6)  $\omega_{i,j} = \pm 1$  – spin at site  $(i, j)$
- (7)  $\omega = (\omega_{1,1}, \omega_{1,2}, \dots, \omega_{N,N})$  – configuration as a matrix of spins
- (8)  $\Omega$  – the set of all possible configurations
- (9)  $E(\omega)$  – magnetic energy of a configuration
- (10)  $H \geq 0$  – the external magnetic field
- (11)  $\langle i, j \rangle$  – the set of 4 sites that are periodic nearest neighbors
- (12)  $k_{\text{Boltz}}$  – Boltzmann constant
- (13)  $\text{Boltz}(\omega) = e^{-E(\omega)/(k_{\text{Boltz}}T)}$  – Boltzmann weight
- (14)  $M(\omega)$  – net spin
- (15)  $\mathbb{E}[M]_T$  – the expected value of  $M(\omega)$
- (16)  $z = \sum_{\omega \in \Omega} e^{-E(\omega)/(k_{\text{Boltz}}T)}$  – the partition function

- (17)  $(i, j)$  – random site in the matrix
- (18)  $\omega'_{(i,j)}$  – flipped sign value at  $(i, j)$
- (19)  $\Delta E$  – change in energy from flip

### 15.6. Sources

Ideas about the Ising model and the associated Metropolis algorithm are adapted from [Hay19, Hay21, Ric10, Sch18]. The exercises are inspired by [Hay21].

### 15.7. Reading Suggestion:

### 15.8. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)

## 15.9. Algorithms and Scripts

**Algorithm.**

**Scripts.**

**R:** R script for complete Ising model.

```

1  ## WARNING: USE ONLY FOR N = 2, 3, 4
2
3  allBinarySeq <- function(N) { # USE ONLY FOR N <= 4!!
4  # list of N copies of -1, 1, simplify=FALSE returns
5  # then all possible combinations of \pm 1 over N
6  # resulting in data.frame of 2^N observations of N
7  # transpose to make N by 2^N matrix
8  # recast back to data.frame
9      as.data.frame(
10         t(
11             expand.grid(
12                 replicate(N, c(-1,1), simplify=FALSE)
13             )
14         )
15     )
16 }
17
18 allConfigs <- function(N) { # USE ONLY FOR N <= 4
19 # returns LIST of all square configs

```

**Data:** Dimension  $N$

**Result:** Plot of magnetization versus normalized temperature near  $T_c$

```

1 function allBinarySeq( $N$ )
2 |   creates all  $2^N$  combinations of  $\pm 1$  over  $N$  places
3 function allConfigs( $N$ )
4 |   creates a list of all possible square configurations of  $\pm 1$  of size  $N \times N$ 
   |   using allBinarySeq( $N*N$ )
5 function energy( $config$ )
6 |   computes magnetization energy
7 function allEnergies
8 |   applies energy function across list of all energies
9 function boltzWeight( $energy$ ,  $kTemp$ )
10 |   computes  $e^{energy*kTemp}$ 
11 function netMag( $config$ )
12 |   computes net magnetization
13 function boltzDist
14 |   computes list of all boltzWeight( $energy$ ,  $kTemp$ )
15 function partitionFunct( $configurations$ ,  $kTemp$ )
16 |   computes sum of all energies using boltzDist( $configurations$ ,  $kTemp$ )
17
18 Set  $J \leftarrow 1$ 
19 Set  $N \leftarrow 3$ 
20 With allConfigs( $N$ ), make a list of all configurations of size  $N \times N$ 
21
22 Set number of normalized temperatures to compute
23 Set a list of normalized temperatures of that length from (2, 2.5) covering
   | the critical value of  $T_c = 2.269$  when  $J = 1$ 
24 Compute the magnetization over all configurations for each of the
   | normalized temperatures
25 Plot the magnetization as a function of normalized temperature

```

**Algorithm 17:** Ising model for magnetization for sizes 2, 3, 4.

```

20 X <- allBinarySeq(N*N)
21 # data.frame of all 2^(N^2) observations over N^2
   # variables
22
23 data = lapply(X, matrix, nrow=N, ncol=N)
24 }
25
26 downConfig <- function(N) { matrix(-1,N,N) } # 1 of 2
   # lowest energy configs
27 upConfig <- function(N) { matrix(1,N,N) } # other
   # lowest energy configs
28

```

**Data:** Dimension  $N$ , normalized temperature, number of sweeps

**Result:** Plot of magnetization after many steps of the Metropolis algorithm

```

1 function Unif( $n$ )
2 |   creates a sample of  $n$  uniform random variables from  $(0, 1)$ 
3 function randomConfig( $N$ )
4 |   creates a random  $N \times N$  configuration of  $\pm 1$ 
5 function boltzWeight( $energy$ ,  $kTemp$ )
6 |   computes  $e^{-energy/kTemp}$ 
7 function surroundNeighbors( $site$ )
8 |   find the 4 periodic surrounding neighbors of  $site$ 
9 function sweepMetropolis( $config$ ,  $N$ )
10 |   for  $x \leftarrow 1 : N$  do
11 |     for  $y \leftarrow 1 : N$  do
12 |        $configAtSite \leftarrow config[x, y]$ 
13 |        $configPrimeAtSite \leftarrow configAtSite * (-1)$ 
14 |        $neigh \leftarrow surroundNeighbors(site)$ 
15 |       Compute  $deltaEnergy$  using  $neigh$ 
16 |       if
17 |          $Unif(1) < \min(1, boltzWeight(deltaEnergy, kTemperature))$ 
18 |         then
19 |            $config \leftarrow configPrime$ 
20 |       end
21 |   end
22
23 Set  $J \leftarrow 1$ ,  $kTemp$ ,  $N$ ,  $mcmcSteps$ 
24 Choose random configuration with randomConfig( $N$ )
25 for  $1 : mcmcSteps$  do
26 |    $config \leftarrow sweepMetropolis(config, N)$ 
27 end
28 Plot image of resulting configuration

```

**Algorithm 18:** Metropolis algorithm applied to Ising model.

```

29  $energy \leftarrow function(config, J=1) \{$  #pass in a
30   MATRIX
31   ## J has units of energy
32   ## Returns a potential energy, negative, with lowest
33   energy  $-4N^2$ 
34   N  $\leftarrow NROW(config)$ 
35
36   below  $\leftarrow config[ c(2:N, 1), ]$ 
37   left  $\leftarrow config[ , c(N, 1:(N-1)) ]$ 
38   above  $\leftarrow config[c(N, 1:(N-1)), ]$ 
39   right  $\leftarrow config[ , c(2:N, 1) ]$ 

```

```

39     nearNeighProd <- config * (below + left + above +
40       right)
41     ## element-wise multiplication, note
42     factorization of sum
43
44     nrg <- -J *sum(nearNeighProd)
45   }
46
47   allEnergies <- function(configurations) { #list of
48     configurations
49     nrgs <- lapply(configurations, energy, J)
50   }
51
52   boltzWeight <- function(nrg, kTemp) { exp(- nrg/kTemp
53     ) }
54
55   netMag <- function(config) { abs( sum( config ) ) }
56
57   boltzDist <- function(configurations, kTemperature)
58   {
59     bzs <- unlist(
60       lapply(allEnergies(configurations),
61         boltzWeight, kTemperature)
62     )
63   }
64
65   partitionFunc <- function(configurations,
66     kTemperature){ #list of energies
67     Z <- sum( boltzDist(configurations,
68       kTemperature) )
69   }
70
71   netSpin <- function(configurations, N) { #list of
72     configurations
73     lm <- lapply(configurations, matrix, N, N)
74     sm <- abs( unlist( lapply(lm, sum) ) ) #absolute
75     value sum of entries in each matrix
76     # unlist converts a list to a vector
77   }
78
79   magnetization <- function(configurations,
80     kTemperature) {
81     Z <- partitionFunc(configurations, kTemperature)
82     mag <- (1/Z) * sum( netSpin(configurations, N) *
83       boltzDist(configurations, kTemperature) )
84   }
85 }

```

```

74 J <- 1
75 N <- 3
76
77 configs <- allConfigs(N)
78
79 nKTemperatures <- 11
80 Temperatures <- seq(2,2.5, length=nKTemperatures)
81 # surrounding the critical value kT_c/J = 2.269 when
   J=1
82
83 m <- rep(0, nKTemperatures)
84
85 for (i in 1:nKTemperatures) {
86   m[i] = magnetization(configs, Temperatures[i])
87   cat("T = ", Temperatures[i], "mag = ", m[i], "\n"
   )
88 }
89
90 plot(Temperatures, m)

```

**R:** R script for Ising Metropolis model.

```

1 randomConfig <- function(N) {
2   config <- matrix(2*sample(0:1, N*N, replace=TRUE)
   -1, N,N)
3 }
4
5 boltzWeight <- function(nrg, kBoltzT) { exp(- nrg/
   kBoltzT) }
6
7 surroundNeighbors <- function(site) {
8   belowSite <- if (site[1] == N) c(1, site[2])
   else c(site[1]+1, site[2])
9   leftSite <- if (site[2] == 1) c(site[1], N)
   else c(site[1], site[2]-1)
10  aboveSite <- if (site[1] == 1) c(N, site[2])
   else c(site[1]-1, site[2])
11  rightSite <- if (site[2] == N) c(site[1], 1)
   else c(site[1], site[2]+1)
12  neighbors <- c(belowSite, leftSite, aboveSite,
   rightSite)
13 }
14
15 sweepMetropolis <- function(config) {
16   for (x in 1:N) {
17     for (y in 1:N) {
18       site <- c(x,y)

```



```

19         configAtSite <- config[ site[1], site[2] ]
20         configPrimeAtSite <- configAtSite * (-1)
21
22         neigh <- surroundNeighbors( site )
23         deltaEnergy <- -2*J * (configPrimeAtSite -
24         configAtSite)*
25             (config[ neigh[1], neigh[2] ] +
26             config[ neigh[3], neigh[4] ] +
27             config[ neigh[5], neigh[6] ]+
28             config[ neigh[7], neigh[8] ]
29             )
30         if ( runif(1) <= min(1, boltzWeight(
31         deltaEnergy, kBoltzT)) )
32         {
33             config[ site[1], site[2] ] <-
34             configPrimeAtSite
35         }
36
37         ## IF deltaEnergy < 0, so energy(configPrime) <
38         energy(config)
39         ## so boltzWeight(deltaEnergy, kBoltzT) > 1,
40         ## THEN runif(1) is certain to be less than p so
41         ## certainly
42         ## change config to configPrime
43         ## ELSE deltaEnergy > 0, so
44         ## energy(configPrime) > energy(config), so
45         ## boltzWeight(deltaEnergy, kBoltzT) < 1,
46         ## so change on chance that runif(1) < p
47         }
48     }
49     return(config)
50 }
51
52 J <- 1
53 N <- 100
54 kBoltzT <- 2.2
55 mcmcSteps <- 50
56
57 config <- randomConfig(N)
58
59 for (i in 1:mcmcSteps ) {
60     config <- sweepMetropolis(config)
61 }
62
63 image(1:N, 1:N, config[N:1, ],
64       col=gray.colors(2),
65       xlab="", ylab="", xaxt="n", yaxt="n")

```

```

61 ## config[N:1, ] so that the plot corresponds to
    matrix order
62 ## i.e. first row of matrix is at top of plot, last
    row at bottom

```

### 15.10. Problems to Work for Understanding

- 1: Show that with random sampling of sites, taking 10,000 steps on a  $100 \times 100$  lattice will miss about  $3,679 \approx 10,000/e$  sites.
- 2: With the nearest neighbor energy model, show that  $\Delta E$  can only have the values  $-16, -8, 0, +8, +16$ . (Use the convention that  $J = 1$ .)
- 3: Compare the Metropolis and Glauber acceptance functions by drawing the graphs of the acceptance probabilities over the range of energy changes  $-17 \leq \Delta E \leq 17$ , one plot with the two functions for each of  $k_{\text{Boltz}}T = 10.0, 2.27, 1.0$ , and  $0.1$ . Draw a dot on each graph at the possible values of  $\Delta T = -16, -8, 0, +8, +16$ .
- 4: Show that for both the Metropolis and Glauber Markov chains, all configurations are accessible, so the chain is irreducible.
- 5: A  $30 \times 30$  grid of squares contains 900 fleas, initially one flea per square. When a bell is rung, each flea independently jumps to a horizontally or vertically adjacent square at random. For most squares, this is one of 4 possibilities, except for fleas in one of the 116 squares on the edge of the grid or at the corners. For edge or corner squares a fleas will jump to one of the 3 or 2 horizontally or vertically adjacent squares. (Note that this is different from the periodic boundary conditions applied to the Ising model.) What is the expected number of unoccupied squares after 50 rings of the bell? Give your answer rounded to six decimal places.



# The Gibbs Sampler

The **Gibbs sampler** is an algorithm for generating random variables from a marginal distribution indirectly, without having to calculate the density. This chapter illustrates the algorithm by exploring several examples. In this chapter, Gibbs sampling is based only on elementary properties of Markov chains.

Mathematically Mature: may contain mathematics beyond calculus with proofs.

## 16.1. Chapter Starter Question

What is Bayes' Rule for 2 jointly distributed continuous random variables  $X$  and  $Y$ ?

## 16.2. General Theory of Gibbs Sampling

Given a joint density  $f(x, y_1, \dots, y_p)$ , the goal is to find characteristics of the marginal density

$$f_X(x) = \int \cdots \int f(x, y_1, \dots, y_p) \, dy_1 \cdots dy_p,$$

such as the mean or variance. Often the integrations are extremely difficult to do, either analytically or numerically. In such cases the Gibbs sampler provides an alternate method for obtaining  $f_X(x)$ .

Gibbs sampling effectively generates a sample  $X_1, \dots, X_m \sim f_X(x)$  without requiring  $f_X(x)$ . By simulating a large enough sample, the mean, variance, or any other characteristic of  $f_X(x)$  can be calculated to the desired degree of accuracy.

First consider the two-variable case. Starting with a pair of random variables  $(X, Y)$ , the Gibbs sampler generates a sample from  $f(x)$  by sampling instead from the conditional distributions  $f(x | y)$  and  $f(y | x)$ . The conditional distributions are often already known in statistical models. This is done by generating a *Gibbs sequence* of random variables

$$(16.1) \quad Y'_0, X'_0, Y'_1, X'_1, Y'_2, X'_2, \dots, Y'_n, X'_n.$$

The first value  $Y'_0 = y'_0$  is specified and the rest of the sequence is obtained iteratively by alternately generating values from

$$\begin{aligned} X'_j &\sim f(x \mid Y'_j = y'_j) \\ Y'_{j+1} &\sim f(y \mid X'_j = x'_j). \end{aligned}$$

The generation of the sequence is **Gibbs sampling**. Under reasonable general conditions, the distribution of  $X'_n$  converges to  $f_X(x)$ , the true marginal of  $X$ , as  $n \rightarrow \infty$ . Thus for  $n$  large enough, the last observation  $X'_n$  is effectively a sample point from  $f_X(x)$ .

### 16.3. Bivariate Binomial Example

This section discusses Gibbs sampling in detail for the simplest case of a  $2 \times 2$  table. Suppose  $X$  and  $Y$  are each marginally Bernoulli random variables with joint distribution (the probabilities  $X$  are by rows, with  $Y = 0$  the first row,  $Y = 1$  the second row)

$$\begin{array}{cc} & X = 0 & X = 1 \\ \begin{array}{c} Y = 0 \\ Y = 1 \end{array} & \left( \begin{array}{cc} p_1 & p_2 \\ p_3 & p_4 \end{array} \right) \end{array}$$

or in terms of the joint probability distribution

$$\begin{pmatrix} f_{X,Y}(0,0) & f_{X,Y}(1,0) \\ f_{X,Y}(0,1) & f_{X,Y}(1,1) \end{pmatrix} = \begin{pmatrix} p_1 & p_2 \\ p_3 & p_4 \end{pmatrix}.$$

The marginal distribution of  $X$  is

$$f_X = (f_X(0), f_X(1)) = (p_1 + p_3, p_2 + p_4),$$

a Bernoulli distribution with success probability  $p_2 + p_4$ . The conditional probabilities can be expressed in two matrices

$$P_{Y|X} = \begin{pmatrix} \frac{p_1}{p_1+p_3} & \frac{p_2}{p_2+p_4} \\ \frac{p_3}{p_1+p_3} & \frac{p_4}{p_2+p_4} \end{pmatrix}$$

and

$$P_{X|Y} = \begin{pmatrix} \frac{p_1}{p_1+p_2} & \frac{p_2}{p_1+p_2} \\ \frac{p_3}{p_3+p_4} & \frac{p_4}{p_3+p_4} \end{pmatrix}$$

where  $P_{Y|X}$  has the conditional probabilities of  $Y$  given  $X$  and  $P_{X|Y}$  has the conditional probabilities of  $X$  given  $Y$ .

As an example, to generate the marginal distribution of  $X$  uses the  $X'$  sequence from (16.1). From  $X'_0$  to  $X'_1$  goes through  $Y'_0$ , so the Gibbs sequence is  $X'_0 \rightarrow Y'_1 \rightarrow X'_1$ . Thus  $X'_0 \rightarrow X'_1$  is a two-stage Markov chain, with transition probability

$$\mathbb{P}[X'_1 \mid X'_0] = \sum_y \mathbb{P}[Y'_1 = y \mid X'_0] \cdot \mathbb{P}[X'_1 \mid Y'_1 = y]$$

For example, to go from  $X = 1$  to  $X = 0$  takes the dot product of the second row of  $P_{Y|X}$  with the first column of  $P_{X|Y}$ . Generally,  $\mathbb{P}[X'_1 \mid X'_0]$  is the right matrix multiplication of  $P_{Y|X}$  by  $P_{X|Y}$ , so

$$P_{X|X} = P_{Y|X} P_{X|Y}$$

is the transition probability matrix for the  $X'$  sequence. Observe carefully the subscript notation, the  $X$ s are “inside”; the  $Y$ s “outside”. The  $Y$ s disappear as the variable of summation from the two-stage Markov chain. The matrix that gives  $\mathbb{P}[X'_n = x_n \mid X'_0 = x_0]$  is  $(P_{X|X})^n$ . Letting  $f_n = (f_n(0), f_n(1))$  denote the marginal probability distribution of  $X'_n$  then  $f_n = f_0 P_{X|X}^n = f_0 (P_{X|X}^{n-1}) P_{X|X} = f_{n-1} P_{X|X}$ . By the Fundamental Theorem for Markov Chains,  $f_n \rightarrow \pi$  as  $n \rightarrow \infty$ , the stationary distribution  $\pi$  satisfying  $\pi P_{X|X} = \pi$ . If the Gibbs sequence converges, the  $\pi$  satisfying  $\pi P_{x|x} = \pi$  must be the marginal distribution of  $X$ . In this small example, it is straightforward to check that  $\pi = (p_1 + p_3, p_2 + p_4)$  satisfies  $\pi P_{X|X} = \pi$ . So stopping the iteration scheme at a large enough value of  $n$  gives random variables distributed approximately as  $\pi$ . The larger the value of  $n$ , the better the approximation. No general guidance on choosing such  $n$  is available. However, one possible approach is to monitor density estimates from  $m$  independent Gibbs sequences, and choosing the first point at which these densities agree to a satisfactory degree.

The algebra for the  $2 \times 2$  case works for any  $n \times m$  joint distribution of  $X$ 's and  $Y$ 's. Analogously define the  $n \times n$  transition matrix  $P_{X|X}$  whose stationary distribution will be the marginal distribution of  $X$ .

If either (or both) of  $X$  and  $Y$  are continuous, then with suitable assumptions, all of the theory still goes through, so the Gibbs sampler still produces a sample from the marginal distribution of  $X$ . The conditional density of  $X_1$  given  $X_0$  is  $f_{X_1|X_0}(X_1 \mid X_0) = \int f_{X_1|Y_1}(x_1 \mid y) f_{Y_1|X_0}(y \mid x_0) dy$ . Then, step by step, write the conditional densities of  $X'_2 \mid X'_0, X'_3 \mid X'_0, X'_4 \mid X'_0, \dots$ . Similar to the  $n$ -step transition matrix  $(P_{x|x})^n$ , derive an “continuous transition probability matrix” with entries satisfying the relationship

$$f_{X'_n|X'_0}(x \mid x_0) = \int f_{X'_n|X'_{n-1}}(X \mid t) f_{X'_{n-1}|X'_0}(t \mid x_0) dt,$$

the continuous version of the right matrix multiplication. As  $n \rightarrow \infty$  it again follows that the stationary distribution is the marginal density of  $X$ , the density to which  $f_{X'_n|X'_0}$ , converges.

## 16.4. Gibbs Sampling from the Bivariate Normal

Recall that the probability density function for the bivariate normal distribution with means 0 and variance 1 for the variables (for simplicity) and correlation  $\rho$  between the two variables is

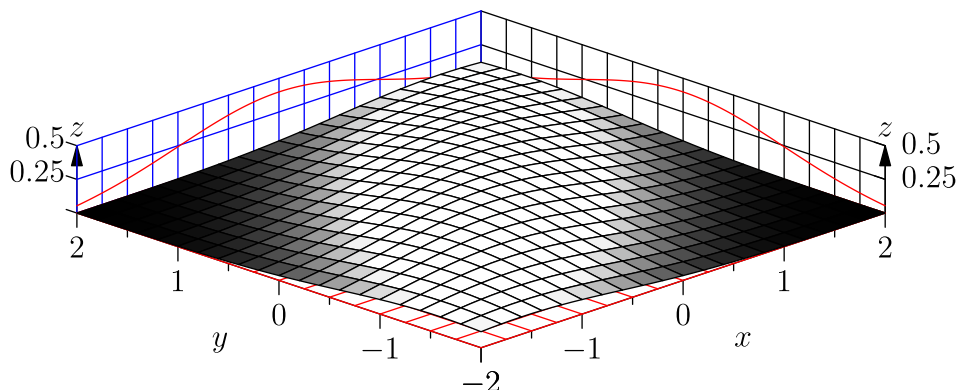
$$f(x, y) = \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)}}.$$

A standard exercise is to show that the marginal densities are in fact

$$f_x(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

and

$$f_y(y) = \frac{1}{\sqrt{2\pi}} e^{-y^2/2}.$$



**Figure 16.1.** Bivariate normal probability density with marginals.

Another standard exercise is to show the conditional probability densities are

$$f_{x|y}(x) = \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-(x-\rho y)^2/(2(1-\rho^2))}$$

and

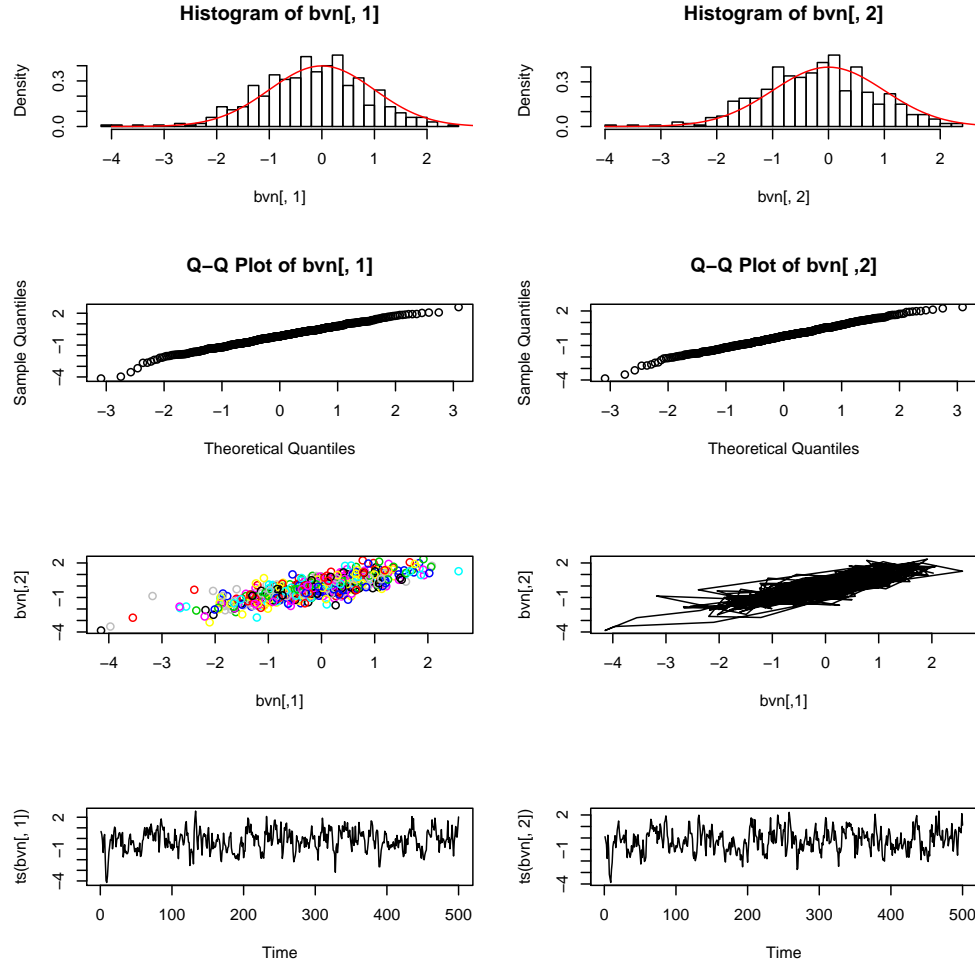
$$f_{y|x}(y) = \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-(y-\rho x)^2/(2(1-\rho^2))}.$$

That is,  $X_i | X_j \sim N(x_j, (1 - \rho^2))$ . Figure 16.1 illustrates the bivariate normal density with  $\rho = 0.8$ . The scaling of the  $z$ -axis is approximately equal to the  $x$  and  $y$  axes, so that the density appears less “hill-like” than is often illustrated. The marginal densities are projected onto coordinate planes at  $x = 2$  and  $y = 2$ .

Because the marginals are known, using the Gibbs sampler is not necessary to simulate them. However, Gibbs sampling using this elementary example is illustrative as in Figure 16.2. Apply the algorithm for 1000 steps. To allow for convergence to the stationary distribution, the first 500 steps are discarded, using only the last 500 steps. The first two subgraphs show the frequencies of the sampled marginal distributions, along with the theoretical densities in red. The correspondence appears close. Better than a visual comparison of the densities is to use a Q-Q plot comparing the sample quantiles to the quantiles of the standard normal distribution. The straight line correspondence of the quantiles over several standard deviations demonstrates the excellent match of simulation to the theoretical density. The third row shows the scatter of the bivariate samples, with the characteristic elliptical distribution. The second figure in the third row shows the autocorrelation of the sample points by connecting successive points with segments. The last two plots illustrate the “white noise”-like aspect of the marginal distributions, as expected. Altogether, these reinforce the intuition that the Gibbs sample has produced a satisfactory sample of the marginal distributions.

### 16.5. A Gibbs Sampler for a Spam Filter

Consider a Bayesian Inference model for an email spam filter. Some algorithm examines each email and classifies the email as *spam* or *not-spam*. The goal is



**Figure 16.2.** Outcomes from Gibbs sampling of a bivariate normal distribution, illustrating the quality of the simulation.

to estimate the prevalence  $\psi$  of email spam without having to directly examine emails and count the instances of email spam. The model has the following random variables and events:

- $[S = 1]$ , the event that the email is in fact spam, a positive outcome occurring with probability  $\mathbb{P}[S = 1] = \psi$ ,
- $[S = 0]$ , the event that the email is *not* spam, a negative outcome with  $\mathbb{P}[S = 0] = 1 - \psi$ ,
- $[R = 1]$ , the event that the algorithm correctly marks spam, a *true positive*,
- $[R = 0]$ , the event that the algorithm *incorrectly* marks spam, a *false negative*.

Then define the following parameters, known or set for the algorithm:



- the *sensitivity* of the algorithm is  $\eta = \mathbb{P}[R = 1 \mid S = 1] = 0.90$  (so the false positive rate is  $\mathbb{P}[R = 0 \mid S = 1] = 0.10$ ),
- *specificity* of the algorithm:  $\theta = \mathbb{P}[R = 0 \mid S = 0] = 0.95$  (so the false negative rate is  $\mathbb{P}[R = 1 \mid S = 0] = 0.05$ ),
- *prevalence*  $\psi = \mathbb{P}[S = 1]$ .

Then

$$\begin{aligned}\tau &= \mathbb{P}[R = 1] = \mathbb{P}[R = 1 \mid S = 1] \mathbb{P}[S = 1] + \mathbb{P}[R = 1 \mid S = 0] \mathbb{P}[S = 0] \\ &= \psi\eta + (1 - \psi)(1 - \theta).\end{aligned}$$

Rewrite the equation to solve for the prevalence  $\psi$ , usually the parameter of interest:

$$\psi = \frac{\tau + \theta - 1}{\eta + \theta - 1}.$$

Assume as an example, that the algorithm marks  $r = 233$  emails as spam out of a total of  $n = 1000$  emails. Then the empirical rate of rejection  $\hat{\tau} = r/n = 0.233$ . From the relation for the prevalence  $\psi$  in terms of the other parameters the empirical estimate of prevalence is  $\hat{\psi} = 0.215$ . Since this is a Bernoulli random variable, the traditional frequentist confidence interval is  $\tau \pm 1.96\sqrt{\tau(1-\tau)/n}$  which becomes  $[0.207, 0.259]$ . Using these in the relation for the prevalence  $\psi$  gives an interval  $\psi \in [0.184, 0.246]$ .

Unfortunately, if  $r$  is relatively small compared to  $n$ , the relation can give nonsensical estimates. For example,  $\eta = 0.99$ ,  $\theta = 0.97$ ,  $r = 5$  from  $n = 250$  gives  $\tau = 0.02$  but  $\psi = -0.0104$ .

Before starting the Gibbs sampling, first use simple Bayesian inference starting from Bayes' Formula

$$\text{Posterior} \propto \text{Prior} \cdot \text{Likelihood}$$

or in probability notation

$$\mathbb{P}[\tau \mid r] \propto \mathbb{P}[\tau] \cdot \mathbb{P}[r \mid \tau].$$

Start with a noninformative prior where  $\tau$  is uniformly distributed on  $(0, 1)$ , but use a Beta density

$$\mathbb{P}[\tau = x] = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}$$

with initial shape parameters  $\alpha = 1$  and  $\beta = 1$  so the density is uniform. Recall that  $\mathbb{P}[r \mid \tau]$  is binomial, so

$$\begin{aligned}\mathbb{P}[\tau \mid r] &\propto (\tau^{\alpha_0-1} (1-\tau)^{\beta_0-1}) \cdot (\tau^r (1-\tau)^{n-r}) \\ &\propto \tau^{\alpha_0+r-1} (1-\tau)^{\beta_0+n-r-1}.\end{aligned}$$

The right side is again the form of the Beta distribution. This correspondence between the Beta families for the prior and the posterior and the Binomials for the likelihood makes them a **conjugate pair**. The mean of the Beta distribution with shape parameters  $\alpha$  and  $\beta$  is  $\alpha/(\alpha+\beta)$  and the variance is  $\alpha\beta/((\alpha+\beta)^2(\alpha+\beta+1))$ .

For the spam classification problem with the previous data

$$\alpha = \alpha_0 + r = 1 + 233 = 234$$

$$\beta = \beta_0 + n - r = 1 + 1000 - 233 = 768.$$

This allows using the resulting Beta density posterior for  $p(\tau | r)$  to derive the mean and confidence interval for  $\tau$ . Using the facts about the mean and variance above, the posterior density mean is  $\alpha/(\alpha + \beta) = 0.234$ . The 95% confidence interval using the Beta c.d.f defined by  $\text{Beta}(\tau_-, \alpha, \beta) = 0.025$  and  $\text{Beta}(\tau_+, \alpha, \beta) = 0.975$  is  $(0.208, 0.260)$ . This is approximately the same as the frequentist confidence interval.

Next use a Gibbs sampler to get point and interval estimates for  $\psi$ . Unlike the estimate for  $\tau$  where the count  $r$  of the spam-marked emails is available, a Gibbs sampler is useful because it is not feasible to directly count the spam emails. Again using Bayes' Formula

$$p = \mathbb{P}[S = 1 | R = 1] = \mathbb{P}[S = 1, R = 1] / \mathbb{P}[R = 1] = \frac{\mathbb{P}[R = 1 | S = 1] \mathbb{P}[S = 1]}{\mathbb{P}[R = 1]} = \psi\eta/\tau$$

and

$$1 - p = \mathbb{P}[S = 1 | R = 0] = \psi(1 - \eta)/(1 - \tau).$$

Simulate the *latent counts*

$$X | (r, \psi) \sim \text{Binom}(r, p)$$

$$Y | (r, \psi) \sim \text{Binom}(n - r, 1 - p)$$

$$\psi | (X, Y) \sim \text{Beta}(\alpha_n, \beta_n)$$

where  $V = X + Y$ ,  $\alpha_n = \alpha_0 + V$  and  $\beta_n = n - V$ . Use one value of  $\psi$  to find the next in the typical Gibbs iteration. This is in effect a Markov chain for which the limiting distribution is the posterior of  $\psi$ . At each iteration, use the prior distribution and the data. The continued and recursive use of this information will cause the convergence of the simulated values toward the appropriate posterior distribution. Figure 16.3 illustrates the results of this Gibbs Sampler method.

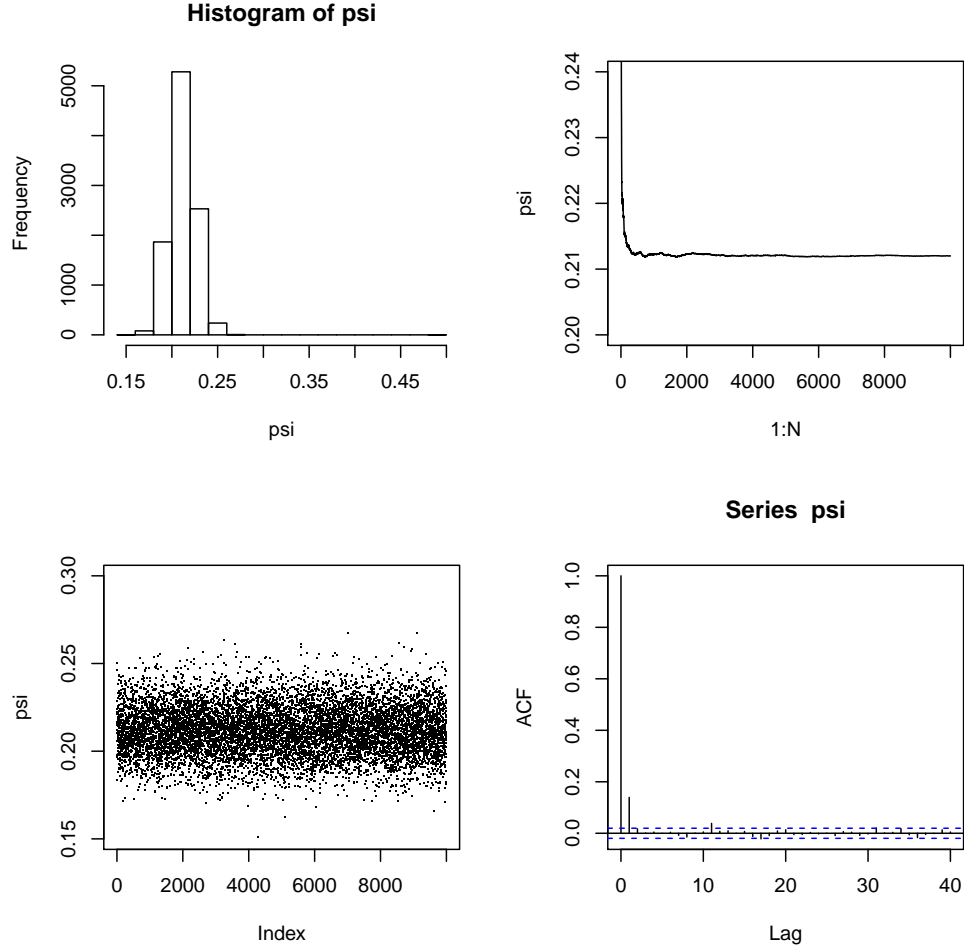
## 16.6. Gibbs Sampling in Statistics

Suppose  $f(x_1, x_2, \dots, x_N)$  is a joint probability density in which the variables represent parameters of a statistical model. The goal is to get point and interval estimates for these parameters. To fit this into the Gibbs sampling framework, assume that all the single-variable conditional probability densities

$$f(x_i | x_j, j \neq i)$$

are available, that is, are a type for which samples can be obtained using standard algorithms. Examples of available densities include the uniform, the normal, the gamma, the Poisson, and any finite distribution. To generate a sequence of samples, select  $\mathbf{x}^0 = (x_1^0, x_2^0, \dots, x_N^0)$  arbitrarily and then create  $\mathbf{x}^1 = (x_1^1, x_2^1, \dots, x_N^1)$  as follows:

- (1) Generate a sample  $x_1^1$  from  $f(x_1 | x_2^0, x_3^0, \dots, x_N^0)$ .
- (2) Generate a sample  $x_2^1$  from  $f(x_2 | x_1^1, x_3^0, x_4^0, \dots, x_N^0)$ .



**Figure 16.3.** Results of the Gibbs sampler applied to the spam filter.

(3) Generate a sample  $x_3^1$  from  $f(x_3 | x_1^1, x_2^1, x_4^0, \dots, x_N^0)$ .

(4) ...

N. Generate a sample  $x_N^1$  from  $f(x_N | x_1^1, x_2^1, \dots, x_{N-1}^1)$ .

One cycle, similar to a sweep of the lattice in the Ising model or a raster scan of an image, produces a new value  $\mathbf{x}^1$ . Repeating this process  $M$  times produces

$$\mathbf{x}^0, \mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^M$$

which approximates a sample from the probability density  $f(x_1, x_2, \dots, x_N)$ .

Using this sample, almost any property of the probability density can be investigated. For example, focusing on only the first component of each  $\mathbf{x}^k$  produces a

sample

$$x_1^0, x_1^1, x_1^2, \dots, x_1^M$$

from the marginal probability distribution of the first component, formally given by the integral

$$f(x_1) = \int_{x_2} \cdots \int_{x_N} f(x_1, x_2, \dots, x_N) \, dx_N \cdots dx_2.$$

In this way, Gibbs sampling can be thought of as a multi-dimensional numerical integration algorithm. The expected value of the first component  $x_1$ ,

$$\mathbb{E}[x_1] = \int_{x_1} x_1 f(x_1) \, dx_1$$

is estimated by the arithmetic mean of the sample  $x_1^0, x_1^1, x_1^2, \dots, x_1^M$ . A 95% confidence interval for  $x_1$  can be taken directly from the sample.

## 16.7. Gibbs Sampling for Normal Parameters

As another example of the Gibbs sampler, suppose that  $X \sim N(\mu, 1/\tau)$  with  $\mu$  and  $\tau$  unknown. Based on a reasonably sized sample, the goal is to get the posterior distributions of  $\mu$  and  $\tau$  using the Gibbs sampler. Here  $\mu$  is the population mean, and  $\tau$ , called the *population precision*, is the reciprocal of the variance,  $n$  is the sample size,  $\bar{x}$  is the sample mean and  $s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2$  is the sample variance. Then make a sequence of iterations  $i = 1, \dots, N$ ; with a sample  $\mu^{(i)}$  from  $f(\mu \mid \tau^{(i-1)}, \text{data})$  (see below for the definition) and sample  $\tau^{(i)}$  from  $f(\tau \mid \mu^{(i-1)}, \text{data})$  (see below for the definition). Then the theory behind Gibbs sampling ensures that after a sufficiently many iterations,  $T$ , the set  $\{(\mu^{(i)}, \tau^{(i)}) : i = T+1, \dots, N\}$  can be seen as a random sample from the joint posterior distribution. The priors are that  $f(\mu, \tau) = f_\mu(\mu) \cdot f_\tau(\tau)$  with  $f_\mu(\mu) \propto 1$  and  $f_\tau(\tau) \propto 1/\tau$ . With these definitions and assumptions, standard theory shows the sample mean from a normal distribution given the population precision has a conditional posterior distribution

$$(\mu \mid \tau, \text{data}) \sim N\left(\bar{x}, \frac{1}{n\tau}\right).$$

Next, the claim is that the precision (the reciprocal of the variance), given the mean, has a conditional posterior distribution

$$(\tau \mid \mu, \text{data}) \sim \text{Gamma}\left(\frac{n}{2}, \frac{2}{(n-1)s^2 + n(\mu - \bar{x})^2}\right).$$

The derivation of the claim is:

$$\text{Posterior} \propto \text{Prior} \cdot \text{Likelihood}$$

or in probability notation

$$\mathbb{P}[\tau \mid \mu, \text{data}] \propto \mathbb{P}[\tau] \cdot \mathbb{P}[\mu, \text{data} \mid \tau].$$

Then using  $\frac{1}{\sigma^n} = \tau^{n/2}$

$$\begin{aligned}
 \mathbb{P}[\tau \mid \mu, \text{data}] &\propto \tau^{-1} \cdot \tau^{n/2} \exp\left(-\frac{\tau}{2} \sum_{\nu=1}^n (x_\nu - \bar{x})^2\right) \\
 &\propto \tau^{-1} \cdot \tau^{n/2} \exp\left(-\frac{\tau}{2} \sum_{\nu=1}^n (x_\nu - \mu + \mu - \bar{x})^2\right) \\
 &\propto \tau^{-1} \cdot \tau^{n/2} \exp\left(-\frac{\tau}{2} \left[ \sum_{\nu=1}^n (x_\nu - \mu)^2 \right. \right. \\
 &\quad \left. \left. + 2 \sum_{\nu=1}^n (x_\nu - \mu)(\mu - \bar{x}) + \sum_{\nu=1}^n (\mu - \bar{x})^2 \right] \right) \\
 &\propto \tau^{-1} \cdot \tau^{n/2} \exp\left(-\frac{\tau}{2} \left[ \sum_{\nu=1}^n (x_\nu - \mu)^2 + \sum_{\nu=1}^n (\mu - \bar{x})^2 \right] \right) \\
 &\propto \tau^{n/2-1} \cdot \exp\left(-\frac{\tau}{2} [(n-1)s^2 + n(\mu - \bar{x})^2]\right).
 \end{aligned}$$

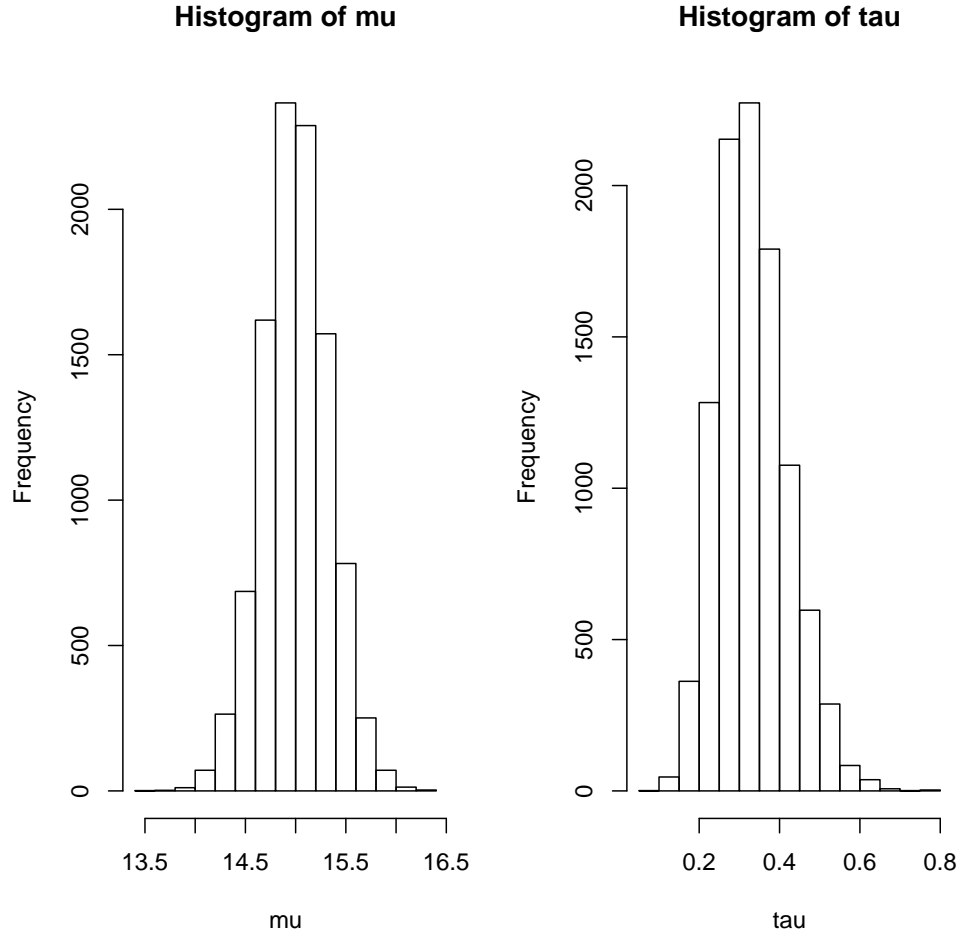
The last expression is now recognizable as a Gamma distribution with shape parameter  $\frac{n}{2}$  and rate (inverse scale parameter)  $(n-1)s^2 + n(\mu - \bar{x})^2$ . Having this distribution is convenient for implementing the Gibbs sampler. (As a side remark, in some derivations for Bayesian statistics, the prior for  $\tau$  is taken to be  $\text{Gamma}(\alpha, \beta)$  which leads to a similar looking Gamma posterior including the additional parameters  $\alpha$  and  $\beta$ , but for Gibbs sampling, this is unnecessary because the theory shows that the sampling will converge even with the simpler choice.)

The R script below implements the Gibbs sampler for these parameters, with  $n = 30$ , a typical value, and postulating  $\bar{x} = 15$ , and  $s^2 = 3$ . The number of iterations is  $N = 11,000$  with a transient period of 1000 iterations. Figure 16.4 shows the results of the of Gibbs sampler for the parameters of a normal distribution.

## 16.8. Bayesian Hierarchical Models

Apply Gibbs sampling formalism to a **Bayesian hierarchical model**. Hierarchical Bayesian models naturally describe the connections among data, observed parameters and other unobserved parameters, sometimes called **latent variables**. A simple three-level hierarchical model uses Bayes' rule to bind together data,  $X$ ; a parameter to be estimated,  $\lambda$ ; and an additional hyper-parameter,  $\beta$ . Both  $\lambda$  and  $\beta$  can be vectors. These are connected in the following way:

- (1) At the first level,  $X$  is described by its likelihood function  $f(X \mid \lambda)$ , the probability of observing  $X$  conditioned on  $\lambda$ .
- (2) At the next level,  $\lambda$  is modeled by a probability density function,  $g(\lambda \mid \beta)$ , conditioned on the parameter  $\beta$ .
- (3) At the third level, the hyper-parameter  $\beta$  is modeled with another density function  $h(\beta)$ . The choice of  $h(\beta)$  reflects the modeler's prior beliefs about the likely values of  $\beta$ .



**Figure 16.4.** Results of the Gibbs sampler for the parameters of a normal distribution.

The three density functions are combined with Bayes' rule, producing a probability density function for  $\lambda$  and  $\beta$  conditioned on the data  $X$

$$F(\lambda, \beta \mid X) \propto f(X \mid \lambda)g(\lambda \mid \beta)h(\beta).$$

The constant of proportionality is the reciprocal of

$$\int_{\lambda} \int_{\beta} f(X \mid \lambda)g(\lambda \mid \beta)h(\beta) \, d\beta \, d\lambda$$

which is independent of the parameters  $\lambda$  and  $\beta$ , though dependent on the data  $X$ . The integrals, (or sums, in the case of discrete distributions) are over all values  $\lambda$  and  $\beta$ . In most cases, the integral or sum is impossible to evaluate. However, as explained before, the Gibbs sampling algorithm avoids this expression.

As a specific example, consider a model of water pump failure rates. The data,  $X$ , are given by pairs  $(s_i, t_i)$  for  $i = 1, 2, \dots, 10$ . Each pair represents failure information for an individual pump. For each pump, assume the number of failures  $s_i$  in time  $t_i$  is given by a Poisson distribution with parameter  $\lambda_i t_i$ , that is

$$f_i(s_i | \lambda_i) = \frac{(\lambda_i t_i)^{s_i} e^{-\lambda_i t_i}}{s_i!}, \quad i = 1, 2, \dots, 10.$$

Assuming the failures occur independently, the likelihood function for  $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_{10})$  is the product:

$$f(X | \lambda) = \prod_{i=1}^{10} \frac{(\lambda_i t_i)^{s_i} e^{-\lambda_i t_i}}{s_i!}.$$

The traditional frequentist approach is to use  $\bar{\lambda}_i = s_i/t_i$  as the point estimate of  $\lambda_i$  for  $i = 1, 2, \dots, 10$ . The Bayesian approach is to assume that the individual  $\lambda_i$ 's are linked together by a common distribution. A natural choice is a gamma distribution with shape parameter  $\alpha$  and scale parameter  $\beta$ , so that the density for the  $i$ th parameter is

$$g_i(\lambda_i | \alpha, \beta) = \frac{\lambda_i^{\alpha-1} e^{-\lambda_i/\beta}}{\beta^\alpha \Gamma(\alpha)}.$$

The remaining hyper-parameter  $\beta$  is described by an inverse gamma distribution with shape parameter  $\gamma$  and scale parameter  $\delta$ , so that

$$h(\beta) = \frac{\delta^\gamma e^{-\delta/\beta}}{\beta^{\gamma+1} \Gamma(\gamma)}.$$

The parameters  $\gamma$  and  $\delta$  are selected to make the top-level inverse gamma reasonably *diffuse*. A diffuse distribution tries to convey as little prior information as possible about the parameters. An extreme case of a noninformative distribution is the uniform distribution on the parameter space.

The resulting posterior joint density for the parameters  $\lambda_1, \lambda_2, \dots, \lambda_{10}$  along with the scale parameter  $\beta$  is

$$F(\lambda_1, \lambda_2, \dots, \lambda_{10}, \beta | X) \propto \left[ \prod_{i=1}^{10} \frac{(\lambda_i t_i)^{s_i} e^{-\lambda_i t_i}}{s_i!} \right] \left[ \prod_{i=1}^{10} \frac{\lambda_i^{\alpha-1} e^{-\lambda_i/\beta}}{\beta^\alpha \Gamma(\alpha)} \right] \left[ \frac{\delta^\gamma e^{-\delta/\beta}}{\beta^{\gamma+1} \Gamma(\gamma)} \right].$$

For  $i = 1, 2, \dots, 10$ , the density for  $\lambda_i$  conditioned on the other parameters is proportional to

$$\lambda_i^{s_i + \alpha - 1} e^{-\lambda_i(t_i + 1/\beta)}.$$

The constant of proportionality is obtained by absorbing all factors independent of  $\lambda_i$ . The form of the density for  $\lambda_i$  shows that  $\mathbb{P}[\lambda_i | \lambda_j, j \neq i, X, \beta]$  is a gamma distribution with shape parameter  $s_i + \alpha$  and scale parameter  $1/(t_i + 1/\beta)$ . Since the gamma distribution is available, Gibbs sampling can be applied at this step. The density for  $\beta$ , conditioned on the other parameters, is proportional to

$$\frac{e^{-(\sum_{i=1}^{10} \lambda_i + \delta)/\beta}}{\beta^{10\alpha + \gamma + 1}}$$

showing that  $\mathbb{P}[\beta \mid \lambda_1, \lambda_2, \dots, \lambda_{10}, X]$  is an inverse gamma distribution with shape parameter  $\gamma + 10\alpha$  and  $\sum_{i=1}^{10} \lambda_i + \delta$ . This too is an available distribution.

This model is an example of a *conjugate hierarchical model*. In a conjugate hierarchical model the intermediate distributions, in this case for  $\lambda_i$  and  $\beta$ , are similar to the original distributions in the hierarchical model. This fits with the Gibbs sampling requirement that these distributions be available.

## 16.9. Gibbs Sampling for Digital Images

A simple model of a digital image consists of pixel elements arranged on a rectangular lattice with  $N$  sites. Each pixel takes a value from a set  $S = \{1, 2, \dots, K\}$ , indicating grayscale or color. For simplicity and analogy to the Ising model, take a black and white image with pixel levels  $-1, +1$ . An image is a configuration  $\omega \in \Omega$  assigning a level to each of the  $N$  sites. Even modestly sized images result in immensely large configuration spaces. For a  $100 \times 100$  black and white image,  $\text{card}(\Omega) = 2^{10,000}$ .

Consider a model for image degradation with additive noise, modeled by  $N$  independent identically distributed random variables  $\mathcal{N} = \{\eta_1, \eta_2, \dots, \eta_N\}$ . Specifically, take noise with the  $\eta_i$  normally distributed with mean 0 and variance  $\sigma^2$ , that is  $\eta_i \sim N(0, \sigma^2)$ . Letting  $\omega^{\text{blurred}}$  indicate the degraded or blurred image,  $\omega^{\text{blurred}} = \omega + \mathcal{N}$ . Since the values of  $\omega^{\text{blurred}}$  are real numbers, the resulting image is determined by rounding each value to the nearest value in  $S$ .

The relationship between the original image and the degraded version is probabilistic, given any image  $\omega$ , there is some probability a particular  $\omega^{\text{blurred}}$  is the degraded version of  $\omega$ . Image reconstruction looks at the problem the other way around; given  $\omega^{\text{blurred}}$ , there is some probability  $\omega$  is the original image. This leads to an application of Bayes' Rule. The *posterior distribution* for  $\omega$  conditioned on  $\omega^{\text{blurred}}$  is

$$\mathbb{P}[\omega \mid \omega^{\text{blurred}}] = \frac{\mathbb{P}[\omega^{\text{blurred}} \mid \omega] \mathbb{P}[\omega]}{\mathbb{P}[\omega^{\text{blurred}}]}.$$

The goal is to find the configuration maximizing  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$ , called the **maximum a posteriori estimate**. The technique is to formulate a new version of the Metropolis algorithm with Gibbs sampling.

By the Law of Total Probability the denominator is

$$\mathbb{P}[\omega^{\text{blurred}}] = \int_{\omega \in \Omega} \mathbb{P}[\omega^{\text{blurred}} \mid \omega] \mathbb{P}[\omega] d\omega.$$

This integral (or sum) is over all  $\omega \in \Omega$  and does not depend on  $\omega$ . This is reminiscent of the partition function and recalling the Metropolis algorithm just ignore it.

The likelihood function  $\mathbb{P}[\omega^{\text{blurred}} \mid \omega]$  is

$$\mathbb{P}[\omega^{\text{blurred}} \mid \omega] \propto \prod_{i=1}^N e^{-\frac{(\omega_i^{\text{blurred}} - \omega_i)^2}{2\sigma^2}} = e^{-\frac{1}{2\sigma^2} \sum_{i=1}^N (\omega_i^{\text{blurred}} - \omega_i)^2}$$

where any constant of proportionality will be absorbed into the denominator above.



An image has patterns which are contiguous regions of similar pixel values. This is reminiscent of the Ising model, where after magnetization the lattice has long-range correlation between pixels, that is, image-like features. On the other hand, if neighboring values reminiscent of the Ising model at high temperatures.

This suggests using the Boltzmann probability distribution with the Ising potential energy function as the prior distribution on images, that is

$$\mathbb{P}[\omega] \propto e^{-E_{\text{ising}}(\omega)/(k_{\text{Boltz}}T)}$$

where

$$E_{\text{ising}}(\omega) = -J \sum_{i=1}^N \sum_{k=1}^4 \omega_i \omega_{\langle i \rangle[k]}$$

is the nearest neighbor affinity. To keep the idea of correlated pixel values, let  $k_{\text{Boltz}}T/J = 1 < T_c$ , the critical temperature below which a phase transition occurs.

Putting all the parts together, the posterior distribution,  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$  is

$$\begin{aligned} \mathbb{P}[\omega \mid \omega^{\text{blurred}}] &\propto e^{-\frac{1}{2\sigma^2} \sum_{i=1}^N (\omega_i^{\text{blurred}} - \omega_i)^2} \cdot e^{-E_{\text{ising}}} \\ &\propto e^{-\left[\frac{1}{2\sigma^2} \sum_{i=1}^N (\omega_i^{\text{blurred}} - \omega_i)^2 + E_{\text{ising}}\right]}. \end{aligned}$$

Viewing this from a statistical mechanics perspective leads to an analog of an energy function

$$\begin{aligned} E_{\text{image}}(\omega \mid \omega^{\text{blurred}}) &= \frac{1}{2\sigma^2} \sum_{i=1}^N (\omega_i^{\text{blurred}} - \omega_i)^2 + E_{\text{ising}} \\ &= \frac{1}{2\sigma^2} \sum_{i=1}^N (\omega_i^{\text{blurred}} - \omega_i)^2 - \sum_{\langle i \rangle[j]} \omega_i \omega_j. \end{aligned}$$

where  $\langle i \rangle$  indicates the set of nearest neighbor sites  $j$  for site  $i$ .

Finding the most probable original image  $\omega$  given  $\omega^{\text{blurred}}$  is equivalent to minimizing  $E_{\text{image}}(\omega \mid \omega^{\text{blurred}})$ . The first term is a positive potential energy penalty for straying too far from the data  $\omega^{\text{blurred}}$  while the second term represents a negative potential energy reflecting the desire to align neighboring pixel values. The optimal solution balances these two conflicting objectives.

Creating an energy function to minimize leads to a contrast in methods. The Ising model starts with an objective function and interprets it as a energy function, using this to convert it to a probability from a physical interpretation. The image reconstruction model starts with a probabilistic situation with a Bayesian structure, leading to an energy function.

To implement Gibbs sampling, the probability of  $\omega_i$  conditioned on *all* the other sites depends on *only* the sites in the nearest neighborhood set. Suppressing the dependence on  $\omega^{\text{blurred}}$ , this means

$$\begin{aligned} \mathbb{P}[\omega_i \mid \omega_j, j \neq i] &= \mathbb{P}[\omega_i \mid \omega_j, j \in \langle i \rangle] \\ &\propto e^{-E_i(\omega_i \mid \omega_j, j \in \langle i \rangle)} \end{aligned}$$

where

$$E_i(\omega_i \mid \omega_j, j \in \langle i \rangle) = \frac{1}{2\sigma^2} (\omega_i^{\text{blurred}} - \omega_i)^2 - \sum_{\langle i \rangle[j]} \omega_i \omega_j.$$

A probability distribution whose conditional probabilities depend on only the values in a neighborhood system is called a **Gibbs distribution** and is an example of a larger notion called a *Markov random field*.

A standard way to implement Gibbs sampling for images is to use a sequence of raster scans, in order by rows or columns, guaranteeing all sites are visited many times. At a selected site  $i$ , select  $\omega_i = k$  with probability

$$\mathbb{P}[\omega_i = \ell] \propto e^{-\frac{1}{2\sigma^2}(\omega_i^{\text{blurred}} - \ell)^2 - \sum_{\langle i \rangle [j]} \ell \omega_j}.$$

Repeating this with many raster scans results in a sequence of images that approximates a sample from the posterior distribution. Note the connection to the previous simple Gibbs sampling algorithm, generating a sample from  $f(x)$  by sampling iteratively from the conditional distributions, except that now there are many more conditional distributions, one for each pixel.

Gibbs sampling fits into the Hastings generalization of the Metropolis algorithm in the following way: In the second step of the Metropolis-Hastings algorithm, the probabilities  $\alpha_{ij}$  are all equal to 1. However, the transitions are no longer time-independent, since each depends on the site choice. As a result, the proof is somewhat more involved than the original proofs of convergence given by Hastings. Gibbs sampling will produce a sequence representing a sample from  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$ . The full algorithm also includes a “temperature” parameter  $T$  to create a simple form of simulated annealing.

**Theorem 16.1.** *Assume*

- (1) *an image with  $N$  pixels,*
- (2)  *$T_k$  is a any decreasing sequence of temperatures such that*
  - (a)  *$T_k \rightarrow 0$  as  $k \rightarrow \infty$ ,*
  - (b)  *$T_k \geq N\Delta / \ln(k)$  for all sufficiently large  $k$  and constant  $\Delta$ .*

*Then starting at  $\omega^{(0)} = \omega^{\text{blurred}}$ , the Gibbs sampling sequence  $\omega^{(k)}$  for  $k = 0, 1, 2, \dots$  converges in distribution to the distribution which is uniform on the minimum vales of  $E_{\text{image}}(\omega)$  and 0 otherwise.*

In other words, following a prescribed annealing schedule, Gibbs sampling must, in theory, produce a maximum a posteriori estimate of  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$ .

Even though this result guarantees convergence to the most likely image, the rate of convergence is slow. Theoretically, for a  $100 \times 100$  lattice with  $N = 10^4$  pixels, using the theorem requires  $e^{20,000}$  steps to go from  $T = 4$  to  $T = 0.5$ . In practice, it takes about 300 – 1000 raster scans to produce acceptable results.

For a black and white ( $k = -1$  or  $1$ ) image Gibbs sampling with annealing is especially straightforward to implement using the ideas of the section on Gibbs sampling. At the pixel  $\omega_i$  define

$$E^k = \frac{1}{2\sigma^2}(k - \omega_i^{\text{blurred}})^2 + k \sum_{\langle i \rangle [j]} \omega_j.$$

Set  $\omega_i = k$  with probability

$$\frac{e^{-E^k / (\text{kBoltz} T)}}{e^{-E^{-1} / (\text{kBoltz} T)} + e^{-E^1 / (\text{kBoltz} T)}}.$$

### 16.10. Chapter Ending Answer

For two continuous random variables  $X$  and  $Y$ , Bayes' rule can be stated in terms of the conditional and marginal densities,

$$f_{X|Y=y}(x) = \frac{f_{X,Y}(x,y)}{f_Y(y)},$$

$$f_{Y|X=x}(y) = \frac{f_{X,Y}(x,y)}{f_X(x)}.$$

Therefore

$$f_{X|Y=y}(x) = \frac{f_{Y|X=x}(y)f_X(x)}{f_Y(y)}.$$

### 16.11. Chapter Summary

#### Key Concepts.

- (1) The Gibbs sampler is an algorithm for generating random variables from a marginal distribution indirectly, without having to calculate the density. Gibbs sampling is based only on elementary properties of Markov chains.
- (2) The simple case of a  $2 \times 2$  table with multinomial sampling clearly illustrates the Markov chain nature of the process.
- (3) The simple case of a bivariate normal density with Gibbs sampling clearly illustrates Gibbs sampling for continuous distributions.
- (4) A simple Bayesian model for a spam filter illustrates typical Gibbs sampling.
- (5) Suppose  $f(x_1, x_2, \dots, x_N)$  is a probability distribution in which the variables represent parameters of a statistical model. Gibbs sampling obtains point and interval estimates for these parameters.
- (6) Suppose  $X \sim N(\mu, 1/\tau)$  with  $\mu$  and  $\tau$  unknown. Based on a reasonably sized sample, Gibbs sampling obtains the posterior distributions of  $\mu$  and  $\tau$ .
- (7) Hierarchical Bayesian models naturally describe the connections among data, observed parameters and other unobserved parameters. A simple three-level hierarchical model uses Bayes' rule to bind together data,  $X$ , a parameter to be estimated,  $\lambda$ , and an additional hyper-parameter,  $\beta$ .
- (8) In image degradation, a version of the Metropolis algorithm called Gibbs sampling the configuration maximizes  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$ , called the maximum a posteriori estimate.

#### Vocabulary.

- (1) The **Gibbs sampler** is a technique for generating random variables from a marginal distribution indirectly, without having to calculate the density.
- (2) **Gibbs sampling** obtains a Gibbs sequence iteratively by alternately generating values from

$$X'_j \sim f(x \mid Y'_j = y'_j)$$

$$Y'_{j+1} \sim f(y \mid X'_j = x'_j).$$

- (3) The functional correspondence between the Beta families for the prior and the posterior and the Binomials for the likelihood makes them a **conjugate pair**.
- (4) **Hierarchical Bayesian models** naturally describe the connections among data, observed parameters and other unobserved parameters, sometimes called **latent variables**. A simple three-level hierarchical model uses Bayes' rule to bind together data,  $X$ , a parameter to be estimated,  $\lambda$ , and an additional hyper-parameter,  $\beta$ .
- (5) The configuration maximizing the probability of a configuration given a randomly changed or blurred configuration,  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$ , is the **maximum a posteriori estimate**.
- (6) A version of the Metropolis algorithm called **Gibbs sampling** maximizes  $\mathbb{P}[\omega \mid \omega^{\text{blurred}}]$ , called the **maximum a posteriori estimate**.
- (7) A probability distribution whose conditional probabilities depend on only the values in a neighborhood system is called a **Gibbs distribution** and is part of a larger notion called a **Markov random field**.

#### Notation.

- (1)  $f(x, y_1, \dots, y_p)$  – a joint density
- (2)  $f_X(x) = \int \dots \int f(x, y_1, \dots, y_p) \, dy_1 \dots dy_p$  – a marginal density
- (3)  $p$  – number of parameters in the joint density
- (4)  $X_1, \dots, X_m \sim f(x)$  – sample from the density  $f(x)$
- (5)  $m$  – number of elements in the sample
- (6)  $(X, Y)$  – Starting pair of random variables
- (7)  $f(x \mid y)$  and  $f(y \mid x)$  – conditional distributions
- (8)  $Y'_0, X'_0, Y'_1, X'_1, Y'_2, X'_2, \dots, Y'_n, X'_n$  – a *Gibbs sequence* of random variables
- (9)  $p_1, p_2, p_3, p_4$  – probabilities in a  $2 \times 2$  table
- (10)  $P_{y|x}$  and  $P_{x|y}$  – conditional probability of  $Y$  given  $X$  and of  $X$  given  $Y$  expressed in matrices
- (11)  $P_{x|x} = P_{y|x}P_{x|y}$  – the transition probability matrix for the  $X'$  sequence
- (12)  $f_n = (f_n(0), f_n(1))$  – the marginal probability distribution of  $X'_n$
- (13)  $\pi$  – stationary distribution satisfying  $\pi P_{x|x} = \pi$
- (14)  $\rho$  – correlation in bivariate normal distribution
- (15)  $[S = 1]$ , the event that the email is in fact spam
- (16)  $[R = 1]$ , the event that a spam email is correctly marked spam, a *true positive*,
- (17)  $\psi$  – probability an email is in fact spam
- (18)  $\eta$  – the false positive rate
- (19)  $\theta$  – the false negative rate
- (20)  $\tau$  – probability that a spam email is correctly marked spam
- (21)  $\alpha, \beta$  – shape parameters for the Beta distribution
- (22)  $f(x_1, x_2, \dots, x_N)$  – a joint probability density in which the variables represent parameters of a statistical model

- (23)  $\vec{x}^0 = (x_1^0, x_2^0, \dots, x_N^0)$ ,  $\vec{x}^1 = (x_1^1, x_2^1, \dots, x_N^1)$  – sequence of samples
- (24)  $X \sim N(\mu, 1/\tau)$  – normal distribution with  $\mu$  the population mean, and  $\tau$  is the population precision
- (25)  $\bar{x}, s^2$  – sample mean and variance
- (26)  $T$  – number of iterations in Gibbs sampling
- (27)  $X$  – parameter to estimate
- (28)  $\lambda, \beta$  – parameter and hyper-parameter in Bayesian hierarchical model
- (29)  $\alpha, \beta, \gamma, \delta$  parameters for distributions

### 16.12. Sources

The sections on the general theory of the Gibbs sampler and the bivariate binomial are adapted from the article “Explaining the Gibbs Sampler” by George Casella and Edward George [CG92]. The section on Gibbs Sampling from the Bivariate Normal is adapted from “A simple Gibbs sampler” by Darren Wilkinson [Wil]. The section on A Gibbs Sampler for a Spam Filter is adapted from “Three Simple Applications of Markov Chains and Gibbs Sampling” by Gui Larangeira [Lar]. The section on theory and Bayesian hierarchical models is adapted from “The Evolution of Markov Chain Monte Carlo Methods” by Richey [Ric10].

### 16.13. Reading Suggestion:

### 16.14. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)

### 16.15. Algorithms and Scripts

**Data:** Number of iterations  $N$ , “Burn in” iterations  $T$ , distributions and parameters

**Result:** Plots of Gibbs sampler results

```

1 Initialize  $X_0, Y_0$ 
2 for  $1 : N$  do
3   | Generate  $X'_j \sim f(x | Y'_j = y'_j)$ 
4   | Generate  $Y'_{j+1} \sim f(y | X'_j = x'_j)$ 
5 end
6 Plot images of resulting distributions and parameters from  $T$  to  $N$ ;
```

**Algorithm 19:** Gibbs sampler algorithm

**Algorithm.**

**Scripts.**

**R:** R script for Gibbs sampler for marginals from bivariate normal.

```

1 gibbs<-function (n, rho)
2 {
3     mat <- matrix(ncol = 2, nrow = n)
4     x <- 0
5     y <- 0
6     mat[1, ] <- c(x, y)
7     for (i in 2:n) {
8         x <- rnorm(1, rho * y, sqrt(1 - rho
9             ^2))
10        y <- rnorm(1, rho * x, sqrt(1 - rho
11            ^2))
12        mat[i, ] <- c(x, y)
13    }
14    mat
15 }
16
17 f <- function(x) { return( (1/sqrt(2 * pi)) * exp(-x
18     ^2/2) )}
19
20 N <- 1000
21 rho <- 0.8
22
23 bvngs <- gibbs(N, rho)
24 bvn <- bvngs[(N/2 + 1):N, ]
25
26 par(mfrow=c(4,2))
27 hist(bvn[,1], freq=FALSE, 40)
28 curve(f, -4, 4, add=TRUE, col="red")
29 hist(bvn[,2], freq=FALSE, 40)
30 curve(f, -4, 4, add=TRUE, col="red")
31 qqnorm(bvn[, 1], main="Q-Q Plot of bvn[, 1]")
32 qqnorm(bvn[, 2], main="Q-Q Plot of bvn[, 2]")
33 plot(bvn, col=1:500)
34 plot(bvn, type="l")
35 plot(ts(bvn[, 1]))
36 plot(ts(bvn[, 2]))
37 par(mfrow=c(1,1))

```

R script for Gibbs sampler for normal parameters.

```

1 # summary statistics of sample
2 n <- 30
3 ybar <- 15
4 s2 <- 3

```

```

5
6 # sample from the joint posterior (mu, tau | data)
7 mu      <- rep(NA, 11000)
8 tau     <- rep(NA, 11000)
9 T       <- 1000      # burnin
10 tau[1] <- 1
11 ## tau[1] <- 1 # initialisation
12 for(i in 2:11000) {
13     mu[i] <- rnorm(n = 1, mean = ybar, sd = sqrt(1 /
14               (n * tau[i - 1])))
15     ## sigmasq[i] <- sigmasq[i-1] * rchisq(n = 1, n-1)
16     / (n - 1)
17     tau[i] <- rgamma(n = 1, shape = n / 2, scale = 2
18               / ((n - 1) * s2 + n * (mu[i] - ybar)^2))
19 }
20 mu <- mu[-(1:T)] # remove burnin
21 tau <- tau[-(1:T)] # remove burnin
22
23 par(mfrow=c(1,2))
24 hist(mu)
25 hist(tau)
26 par(mfrow=c(1,1))

```

R script for Gibbs sampler for estimating spam prevalence.

```

1 N <- 10000      # Number of iterations
2 Nb <- 2000; N1 <- N+1 # Burn-in
3
4 psi <- numeric(N)
5 psi[1] <- .5      # Initial value
6
7 alpha.0 <- 1.0
8 beta.0 <- 1.0
9 eta <- 0.99
10 theta <- 0.97
11 r <- 233
12 n <- 1000
13
14 for(i in 2:N) {      # Gibbs Sampler Loop
15     tau <- psi[i-1]*eta+(1-psi[i-1])*(1-theta)
16     X <- rbinom(1, r, psi[i-1]*eta/tau)
17     Y <- rbinom(1, n-r, psi[i-1]*(1-eta)/(1-tau))
18     psi[i] <- rbeta(1, alpha.0+X+Y, beta.0+n-X-Y)
19 }
20
21 gspsi <- mean(psi[Nb:N])
22

```

```

23 par(mfrow=c(2,2))
24 hist(psi)
25 plot(1:N,cumsum(psi)/(1:N),type="l",ylab="psi",ylim
      =c(0.20,0.24))
26 plot(psi,type='p',pch='.',ylim=c(0.15,0.30))
27 acf(psi)

```

### 16.16. Problems to Work for Understanding

- R:** 1: For the simplest case where  $X$  and  $Y$  are each marginally Bernoulli random variables with joint distribution

$$\begin{array}{cc} & X = 0 & X = 1 \\ \begin{array}{c} Y = 0 \\ Y = 1 \end{array} & \left( \begin{array}{cc} p_1 & p_2 \\ p_3 & p_4 \end{array} \right) \end{array}$$

show that  $f = (p_1 + p_3, p_2 + p_4)$  satisfies  $fP_{X|X} = f$ .

- 2: The probability density function for the bivariate normal distribution with means 0 and variance 1 for the variables and correlation  $\rho$  between the two variables is

$$f(x, y) = \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)}}.$$

Show that the  $x$  marginal is

$$f_x(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

- 3: The probability density function for the bivariate normal distribution with means 0 and variance 1 for the variables and correlation  $\rho$  between the two variables is

$$f(x, y) = \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)}}.$$

Show that the  $x$  conditional given  $y$  is

$$f_{x|y}(x | y) = \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{(x-\rho y)^2}{2(1-\rho^2)}}.$$





## Gibbs Sampling, Eigen Decompositions, and Spectral Bounds for Markov Chains

This chapter closely examines the spectral approach to convergence of Markov chains to a stationary distribution. The spectral approach uses eigenfunction decompositions to estimate distance measures and inequalities for probability distributions. The focus is on two-component Gibbs samplers, with applications to the Beta/Binomial and Poisson/Gamma Gibbs samplers. These two-component Gibbs samplers lead to decompositions in terms of orthogonal polynomials. Finally, the results for the Poisson/Gamma Gibbs samplers leads to a convergence rate for a specific Markov chain birth and immigration model.

Mathematicians Only: prolonged scenes of intense rigor.

### 17.1. Chapter Starter Question

Recall the magical land of Oz where the weather follows a pattern. If it is raining today, then tomorrow has a 50% chance of raining again, and a 25% chance of either having a nice day or a snowy day tomorrow. Similarly if it is snowing, the next day has a 50% chance of again having snow, and a 25% chance of either having a nice day, or a rainy day. Also the land of Oz never has two nice days in a row, and equally has rain or snow the day after a nice day. Recall that for  $P^n$ , for large values of  $n$ , the row vectors approach the stationary distribution  $\pi = (2/5, 1/5, 2/5)$ . Starting from the state of rain, find the Euclidean distance of the state at day  $n$  from the stationary distribution, using the eigenvalues and eigenvectors of the transition probability matrix.

### 17.2. Notation and Assumptions

- Let  $\mathcal{X}$  be a state space, either finite or infinite.

- Let  $\mu(dx)$  be a reference measure on  $\mathcal{X}$ , typically Lebesgue measure or counting measure.
- Let  $m(x)$  be a probability density with respect to  $\mu$ , meaning  $m(x) \geq 0$  and  $\int_{\mathcal{X}} m(x)\mu(dx) = 1$ .
- Let  $P(x, dy)$  be a Markov kernel on  $\mathcal{X}$ . This means that for each  $x$ ,  $P(x, \cdot)$  is a probability measure on  $\mathcal{X}$ .
- Then  $P$  creates a Markov chain  $X_0, X_1, X_2, \dots$  with starting state  $X_0 = x$  by choosing  $X_1$  with  $P(x, \cdot)$ , choosing  $X_2$  with  $P(X_1, \cdot)$  and so on.
- Recall that the Markov chain is reversible if  $P$  operating on  $L^2(m)$  by  $P[f](x) = \int f(y)P(x, dy)$  is self-adjoint,  $\langle Pf, g \rangle = \langle f, Pg \rangle$ .
- Often the Markov kernel has the density form  $P(x, dy) = p(x, y)\mu(dy)$  and reversibility reduces to  $m(x)p(x, y) = m(y)p(y, x)$  for all  $x, y$ . Reversibility says the Markov chain run forward is the same as the chain run backward, in analogy with the time reversibility of the laws of mechanics. Here  $P$  operates on all of  $L^2(m)$ , so reversible Markov kernels are bounded self-adjoint operators.
- Suppose  $P$  has a square integrable kernel, so that  $P$  operating on  $L^2(m)$  becomes  $P[f](x) = \int f(y)p(x, y)\mu(dy)$ .
- Then  $P$  is compact and by the Spectral Theorem there are eigenvalues  $\lambda_\nu$  and corresponding eigenvectors  $f_\nu$  so that  $Pf_\nu = \lambda_\nu f_\nu$  for  $\nu = 0, 1, 2, \dots$
- Under a mild connectedness condition,  $\lambda_0 = 1$ ,  $f_0 = 1$  and  $1 = \lambda_0 > \lambda_1 \geq \lambda_2 \geq \dots \geq -1$ .
- Then the kernel can be written

$$p(x, y) = m(x) \sum_{\nu=0}^{\infty} \lambda_\nu f_\nu(x) f_\nu(y).$$

In a specific simple example, for finite state spaces with counting measure, this says the transition probability matrix is symmetric.

- The iterated kernel is

$$p^n(x, y) = m(x) \sum_{\lambda=0}^{\infty} \lambda_\nu^n f_\nu(x) f_\nu(y).$$

If  $f_\nu(x)$  and  $f_\nu(y)$  are bounded, then using  $f_0 \equiv 1$ ,

$$p^n(x, y) \rightarrow m(y), \text{ as } n \rightarrow \infty.$$

The goal is to provide useful information about the rate of convergence, that is, to provide a quantitative bound on how large  $n$  must be to have  $\|P_x^n - m\| < \epsilon$ . To use this representation, good information on  $\lambda_i$  and  $f_i$  must be available. For an example, see the chapters on Convergence to Stationary and Fastest Mixing.

### 17.3. Two-Component Gibbs Sampling

Let  $(\mathcal{X}, \mathcal{F})$  be a measurable space equipped with a  $\sigma$ -finite measure  $\mu(dx)$  on  $\mathcal{F}$ . Let  $(\Theta, \mathcal{G})$  be a measurable space equipped with a probability measure  $\pi(d\theta)$  on  $\mathcal{G}$ . (Here  $\pi(d\theta)$  is the probability distribution on the parameter, not the stationary

distribution.) The measure on the  $(\Theta, \mathcal{G})$  space is the *prior distribution* or just the *prior* for short. In many classical situations the prior is given by a density  $g(\theta)$  with respect to the Lebesgue measure  $d\theta$  so  $\pi(d\theta) = g(\theta) d\theta$ , but there are also examples where the parameter  $\theta$  is discrete, which cannot be described with a density. Thus, it is necessary to work with general prior probabilities  $\pi(d\theta)$  throughout. Let  $\{f_\theta(x) : \theta \in \Theta\}$  be a family of probability densities on  $\mathcal{X}$  with respect to the  $\sigma$ -finite measure  $\mu(dx)$ . Together these measures define a probability measure on  $\mathcal{X} \times \Theta$  via

$$\mathbb{P}[A \times B] = \int_B \int_A f_\theta(x) \mu(dx) \pi(d\theta), \quad A \in \mathcal{F}, B \in \mathcal{G}.$$

The *marginal density* on  $\mathcal{X}$  is

$$m(x) = \int_\Theta f_\theta(x) \pi(d\theta)$$

so

$$\int_{\mathcal{X}} m(x) \mu(dx) = 1.$$

Assume  $0 < m(x) < \infty$  for every  $x \in \mathcal{X}$ . The *posterior density* with respect to  $\pi(d\theta)$  is

$$\pi(\theta | x) = f_\theta(x) / m(x).$$

The probability  $\mathbb{P}[\cdot]$  splits with respect to the measure  $m(dx)$  defined by  $m(dx) = m(x) \mu(dx)$  in the form

$$\mathbb{P}[A \times B] = \int_A \int_B \pi(\theta | x) \pi(d\theta) m(dx), \quad A \in \mathcal{F}, B \in \mathcal{G}.$$

The **systematic scan Gibbs sampler** for drawing from the distribution  $\mathbb{P}[\cdot]$  proceeds as follows. Starting from  $(x, \theta)$ , first, draw  $x'$  from  $f_\theta(\cdot)$ ; second, draw  $\theta'$  from  $\pi(\cdot | x')$ . The output is  $(x', \theta')$ . This generates a Markov chain  $(x, \theta) \rightarrow (x', \theta') \rightarrow \dots$  having kernel

$$K(x, \theta; x', \theta') = f_\theta(x') \cdot f_{\theta'}(x') / m(x')$$

with respect to  $\mu(dx') \pi(d\theta)$ . Note that the kernel does not depend on  $x$ .

A slight variant exchanges the order of the draws: Starting from  $(x, \theta)$ , first, draw  $\theta'$  from  $\pi(\cdot | x)$ ; second, draw  $x'$  with density  $f_{\theta'}(\cdot)$ . The output is  $(x', \theta')$ . This generates a Markov chain  $(x, \theta) \rightarrow (x', \theta') \rightarrow \dots$  having kernel

$$\tilde{K}(x, \theta; x', \theta') = \pi(\theta' | x) \cdot f_{\theta'}(x') = f_{\theta'}(x) / m(x) \cdot f_{\theta'}(x') = f_{\theta'}(x') \cdot f_{\theta'}(x) / m(x)$$

with respect to  $\mu(dx') \pi(d\theta)$ . Note that the kernel does not depend on  $\theta$ .

Under mild conditions these two chains have stationary distribution  $\mathbb{P}[\cdot]$ .

The ***x-chain*** is: first, draw  $\theta'$  with probability  $\pi(\theta' | x)$ ; second,  $x'$  with probability  $f_{\theta'}(x')$  (with the abuse of notation that the probability is given by the density function  $f_{\theta'}(x')$ ). The *x-chain* has transition kernel

$$k(x, x') = \int_\Theta \pi(\theta | x) f_\theta(x') \pi(d\theta) = \int_\Theta \frac{f_\theta(x) \cdot f_\theta(x')}{m(x)} \pi(d\theta).$$

Note that  $\int_{\mathcal{X}} k(x, x') \mu(dx') = 1$  so that  $k(x, \cdot)$  is a probability density with respect to  $\mu$ . Note further that  $m(x)k(x, x') = m(x')k(x', x)$  so that the  $x$ -chain has  $m(dx)$  as a stationary distribution.

The  **$\theta$ -chain** is: first draw  $x$  from  $f_{\theta}(x)$  and then  $\theta'$  from  $\pi(\theta' | x)$ . The  $\theta$ -chain has transition kernel

$$k(\theta, \theta') = \int_{\mathcal{X}} f_{\theta}(x) \pi(\theta' | x) \mu(dx) = \int_{\mathcal{X}} \frac{f_{\theta}(x) f_{\theta'}(x)}{m(x)} \mu(dx).$$

Note  $\int k(\theta, \theta') \pi(d\theta') = 1$  so that  $k(\theta, \theta')$  is a probability density with respect to  $\pi$ . Additionally  $k(\theta, \theta')$  has  $\pi(d\theta)$  as reversing measure.

The **random scan chain** proceeds as follows. From  $(x, \theta)$ , pick a coordinate at random equally, and update it from the appropriate conditional distribution. Then formally, for  $g \in L^2(\mathbb{P})$

$$(17.1) \quad \bar{K}g(x, \theta) = \frac{1}{2} \int_{\Theta} g(x, \theta') \pi(\theta' | x) \pi(d\theta') + \frac{1}{2} \int_{\mathcal{X}} g(x', \theta) f_{\theta}(x') \mu(dx').$$

Note three things about the random scan chain.

- (1)  $\bar{K}$  sends  $L^2(\mathbb{P}) \rightarrow L^2(\mathbb{P})$  and is reversible with respect to  $\mathbb{P}$ . This is a reason for using the random scans.
- (2) The right side of equation 17.1 is the sum of a function of  $x$  alone and a function of  $\theta$  alone. Then  $\bar{K} : L^2(\mathbb{P}) \rightarrow L^2(m) + L^2(\pi)$ , that is, the range of  $\bar{K}$  is contained in  $L^2(m) + L^2(\pi)$ .
- (3) If  $\bar{K} \in (L^2(m) + L^2(\pi))^{\perp}$ , then  $\bar{K} = 0$ , or  $(L^2(m) + L^2(\pi))^{\perp} \subseteq \text{Ker } \bar{K}$ . In more detail, for  $h \in L^2(\mathbb{P})$ ,

$$\langle \bar{K}g, h \rangle_{\mathbb{P}} = \int (\bar{K}g) \cdot h \, d\mathbb{P} = \int (\bar{K}h) \cdot g \, d\mathbb{P} = 0.$$

Thus,  $\bar{K}g = 0$

**Example 17.1.** The Poisson/Exponential distributions. Let  $\mathcal{X} = \{0, 1, 2, 3, \dots\}$ ,  $\mu(dx)$  is counting measure,  $\Theta = (0, \infty)$ ,  $f_{\theta}(x) = e^{-\theta} \theta^x / x!$ . Take  $\pi(d\theta) = e^{-\theta} d\theta$ . By the definition of the Gamma integral (see the exercises)

$$m(x) = \int_0^{\infty} \frac{e^{-\theta} \theta^x}{x!} e^{-\theta} d\theta = \int_0^{\infty} \frac{e^{-2\theta} \theta^x}{x!} d\theta = \frac{1}{2^{x+1}}.$$

The posterior distribution with respect to  $\pi(d\theta)$  is  $\pi(\theta | x) = f_{\theta}(x)/m(x) = 2^{x+1} e^{-\theta} \theta^x / x!$ . The  $x$ -chain has kernel (see the exercises)

$$\begin{aligned} k(x, x') &= \int_0^{\infty} \frac{2^{x+1} \theta^x e^{-\theta}}{x!} \cdot \frac{\theta^{x'} e^{-\theta}}{x'!} \cdot e^{-\theta} d\theta \\ &= \int_0^{\infty} \frac{2^{x+1} \theta^{x+x'} e^{-3\theta}}{x! x'!} d\theta = \frac{2^{x+1}}{3^{x+x'+1}} \binom{x+x'}{x}, \quad x, x' \in \{0, 1, 2, 3, \dots\}. \end{aligned}$$

The  $\theta$ -chain has kernel

$$\begin{aligned} k(\theta, \theta') &= \int_{\mathcal{X}} \frac{f_{\theta}(x) f_{\theta'}(x)}{m(x)} \mu(dx) \\ &= \sum_{x=0}^{\infty} \frac{e^{-\theta} \theta^x}{x!} \cdot \frac{e^{-\theta'} (\theta')^x}{x!} \cdot 2^{x+1} = 2e^{-\theta-\theta'} \sum_{x=0}^{\infty} \frac{(2\theta\theta')^x}{(x!)^2} = 2e^{-\theta-\theta'} I_0(\sqrt{8\theta\theta'}) \end{aligned}$$

with respect to  $\pi(d\theta)$ , where  $I_0$  is the classical modified Bessel function. Following Feller [Fel71, Section 2.7, pages 58–61], the series definition of the modified Bessel function of order 0 is

$$I_0(z) = \sum_{\nu=0}^{\infty} \frac{1}{(\nu!)^2} \left(\frac{z}{2}\right)^{2\nu}.$$

▽

**Distances and Inequalities.** This section recalls some general results to apply to the two-component Gibbs sampler chains or the  $x$ -chain and  $\theta$ -chain.

Consider a Markov chain described by its kernel  $K(\xi, \xi')$  with respect to a measure  $\tilde{\mu}(d\xi')$ . For example, for the two-component sampler, the Markov chain states would be  $\xi = (x, \theta)$  with respect to the product measure  $\tilde{\mu}(d\xi) = \mu(dx)\pi(d\theta)$ . As another example, for the  $x$ -chain the Markov chain states would be  $\xi = x$  with respect to measure  $\tilde{\mu}(d\xi) = \mu(dx)$ . Suppose further that the chain has stationary measure  $m(d\xi) = m(\xi)\tilde{\mu}(d\xi)$  (that is,  $m(\xi)$  is a density for the stationary distribution) and write

$$\begin{aligned} \hat{K}(\xi, \xi') &= K(\xi, \xi')/m(\xi') \\ \hat{K}_{\xi}^{\ell}(\xi') &= \hat{K}^{\ell}(\xi, \xi') = K^{\ell}(\xi, \xi')/m(\xi') \end{aligned}$$

for the kernel and iterated kernel of the chain with respect to the stationary measure  $m(d\xi)$ , where the superscript  $\ell$  denotes the chain after  $\ell$  steps.

The **chi-square distance** between the distribution of the chain started at  $\xi$  after  $\ell$  steps and its stationary measure is

$$\chi_{\xi}^2(\ell) = \int \left| \hat{K}_{\xi}^{\ell}(\xi') - 1 \right|^2 m(d\xi') = \int \frac{|K^{\ell}(\xi, \xi') - m(\xi')|^2}{m(\xi')} \tilde{\mu}(d\xi').$$

Recall the definition of the total variation distance between the iterated kernel of the chain  $K^{\ell}(\xi, \xi')$  and the stationary distribution  $m(d\xi)$

$$\|K_{\xi}^{\ell} - m\|_{TV} = \frac{1}{2} \int \left| \hat{K}_{\xi}^{\ell}(\xi') - 1 \right| m(d\xi') = \frac{1}{2} \int |K^{\ell}(\xi, \xi') - m(\xi')| \tilde{\mu}(d\xi').$$

By Jensen's Inequality the chi-square distance gives an upper bound on the total variation distance, namely

$$4\|K_{\xi}^{\ell} - m\|_{TV}^2 \leq \chi_{\xi}^2(\ell).$$

### 17.4. Lemmas on Convergence Rates

Analysis of the rate of convergence comes from eigenfunction decompositions. A function  $\phi$  such that

$$\begin{aligned} K[\phi(\xi)] &= \int K(\xi, \xi') \phi(\xi') \tilde{\mu}(d\xi') = \lambda \phi(\xi), \\ m(\phi) &= \int 1 \cdot \phi(\xi) m(\xi) \tilde{\mu}(d\xi) = 0 \end{aligned}$$

for a complex number  $\lambda$  is a generalized eigenfunction with eigenvalue  $\lambda$ . The eigenfunction is “generalized” because there is no assumption  $\phi$  belongs to a specific  $L^2$  space, just that  $K[\phi]$  and  $m(\phi)$  can be computed. The second condition, orthogonality to constants in  $L^2(m)$  will be automatically satisfied when  $|\lambda| < 1$ . Such an eigenfunction yields a simple lower bound on the convergence of the chain to its stationary measure.

**Lemma 17.2.** *Let  $p \in [1, \infty]$ .*

(1) *For the  $x$ -chain*

$$\begin{aligned} \|K_{x,\theta}^\ell / f - 1\|_{p,\mathbb{P}}^p &\leq \int \|\hat{k}_z^{\ell-1} - 1\|_{p,m}^p f_\theta(z) \mu(dz) \\ &\leq \sup_z \|\hat{k}_z^{\ell-1} - 1\|_{p,m}^p \end{aligned}$$

and

$$\|\tilde{K}_{x,\theta}^\ell / f - 1\|_{p,\mathbb{P}}^p \leq \|\hat{k}_x^{\ell-1} - 1\|_{p,m}^p.$$

(2) *For the  $\theta$ -chain*

$$\begin{aligned} \|\tilde{K}_{x,\theta}^\ell / f - 1\|_{p,\mathbb{P}}^p &\leq \int \|k_\theta^{\ell-1} - 1\|_{p,\pi}^p \pi(\theta | x) \pi(d\theta) \\ &\leq \sup_\theta \|k_\theta^{\ell-1} - 1\|_{p,\pi}^p \end{aligned}$$

and

$$\|K_{x,\theta}^\ell / f - 1\|_{p,\mathbb{P}}^p \leq \|k_\theta^{\ell-1} - 1\|_{p,\pi}^p.$$

**Proof.** (1) Recall the bivariate chain has transition density

$$K(x, \theta; x', \theta') = f_\theta(x') f_{\theta'}(x') / m(x').$$

By direct computation

$$K^\ell(x, \theta; x', \theta') = \int f_\theta(z) k^{\ell-1}(z, x') \frac{f_{\theta'}(x')}{m(x')} \mu(dz).$$

(2) For the variant  $\tilde{K}$ , the similar formula reads

$$\tilde{K}^\ell(x, \theta; x', \theta') = \int k^{\ell-1}(x, z) \frac{f_{\theta'}(z)}{m(z)} f_{\theta'}(x') \mu(dz).$$

(3) These two bivariate chains have stationary density  $f(x, \theta) = f_\theta(x)$  with respect to the measure  $\mu(dx) \cdot \pi(d\theta)$ . So write

$$\frac{K^\ell(x, \theta; x', \theta')}{f(x', \theta')} - 1 = \int (\hat{k}^{\ell-1}(z, x') - 1) f_\theta(z) \mu(dz)$$

and

$$\frac{\tilde{K}^\ell(x, \theta; x', \theta')}{f(x', \theta')} - 1 = \int (\hat{k}^{\ell-1}(x, z) - 1) f_{\theta'}(z) \mu(dz).$$

- (4) To prove the second inequality in the lemma (the proof of the first is similar), write

$$\begin{aligned} & \|\tilde{K}_{x,\theta}^\ell / f - 1\|_{p,\mathbb{P}}^p \\ &= \iint \left| \int (\hat{k}^{\ell-1}(x, z) - 1) f_{\theta'}(z) \mu(dz) \right|^p \cdot f_{\theta'}(x') \mu(dx') \pi(d\theta') \\ &\leq \iint \int \left| (\hat{k}^{\ell-1}(x, z) - 1) \right|^p f_{\theta'}(z) \mu(dz) \cdot f_{\theta'}(x') \mu(dx') \pi(d\theta') \\ &= \int \left| (\hat{k}^{\ell-1}(x, z) - 1) \right|^p m(z) \mu(dz) \\ &= \int \left| (\hat{k}^{\ell-1}(x, z) - 1) \right|^p m(dz). \end{aligned}$$

□

The following is the proof of the lower bound.

**Lemma 17.3.** *Consider  $g$  as a function of  $x$  only, with the abuse of notation  $g(x, \theta) = g(x)$ . Then*

$$\tilde{K}g(x, \theta) = \int k(x, x') g(x') \mu(dx').$$

**Proof.** Assume  $g(x, \theta) = g(x)$ , then

$$\tilde{K}g(x, \theta) = \iint \frac{f_{\theta'}(x) f_{\theta'}(x')}{m(x)} g(x') \mu(dx') \pi(d\theta') = \int k(x, x') g(x') \mu(dx').$$

□

**Lemma 17.4.** (1) *Let  $\chi_{x,\theta}^2(\ell)$  and  $\tilde{\chi}_{x,\theta}^2(\ell)$  be the chi-square distances after  $\ell$  steps for the  $K$ -chain and the  $\tilde{K}$ -chain, respectively, starting at  $(x, \theta)$ .*

- (2) *Let  $\chi_x^2(\ell)$ ,  $\chi_\theta^2(\ell)$  be the chi-square distance for the  $x$ -chain starting at  $x$  and the  $\theta$ -chain starting at  $\theta$ .*

Then

(1)

$$\begin{aligned} \chi_x^2(\ell) &\leq \tilde{\chi}_{x,\theta}^2(\ell) \leq \chi_x^2(\ell - 1) \\ \|k_x^\ell - m\|_{TV} &\leq \|\tilde{K}_{x,\theta}^\ell - f\|_{TV} \leq \|k_x^{\ell-1} - m\|_{TV}. \end{aligned}$$

(2)

$$\begin{aligned} \chi_\theta^2(\ell) &\leq \tilde{\chi}_{x,\theta}^2(\ell) \leq \chi_\theta^2(\ell - 1) \\ \|k_\theta^\ell - 1\|_{TV} &\leq \|K_{x,\theta}^\ell - f\|_{TV} \leq \|k_x^{\ell-1} - 1\|_{TV}. \end{aligned}$$

**Proof.** This is immediate from the previous lemmas.

□



**Eigenvalues and Eigenfunctions.** The results of this section show common Gibbs sampler Markov chains have polynomial eigenvectors, with explicitly known eigenvalues. This includes the  $x$ -chain,  $\theta$ -chain and the random scan chain.

Let  $k = \text{card}(\text{supp}(m(x)))$ , where  $m(x)$  is the marginal density on  $\mathcal{X}$ ,  $m(x) = \int_{\Theta} f_{\theta}(x) \pi(d\theta)$ . Using here the notation  $k$  is consistent with the convention that the number of states in a Markov chain is  $k$ , not to be confused with the Markov kernels previously. The value of  $k$  may be finite or infinite. To be definite in this section, assume the support of  $\pi$  is infinite. Moreover, make the following hypotheses.

**H1::** For some  $\alpha_x > 0$  and  $\alpha_{\theta} > 0$ ,

$$\int e^{\alpha_x |x| + \alpha_{\theta} |\theta|} d\mathbb{P} < \infty.$$

**H2::** For  $0 \leq \nu < k$ , the  $\nu$ th moment  $\mathbb{E}_{\theta} [X^{\nu}]$  is a polynomial in  $\theta$  of degree  $\nu$  with leading coefficient  $\eta_{\nu} > 0$ .

**H3::** For  $\nu \geq 0$ , the  $\nu$ th moment  $\mathbb{E}_x [\theta^{\nu}]$  is a polynomial in  $x$  of degree  $\nu$  with leading coefficient  $\mu_{\nu} > 0$ .

By (H1),  $L^2(m(dx))$  admits a unique orthogonal basis of monic polynomials  $p_{\nu}$ ,  $0 \leq \nu < \infty$ , with  $p_{\nu}$  having degree  $\nu$ . Also,  $L^2(\pi(d\theta))$  admits a unique orthogonal basis of monic polynomials  $q_{\nu}$ ,  $0 \leq \nu < \infty$ , with  $q_{\nu}$  of degree  $\nu$ . As usual,  $\eta_0 = \mu_0 = 1$  and  $p_0 \equiv q_0 \equiv 1$ .

**Theorem 17.5.** Assume (H1)–(H3), then

- (1) The  $x$ -chain has eigenvalues  $\lambda_{\nu} = \eta_{\nu} \mu_{\nu}$  with eigenvectors  $p_{\nu}$ ,  $0 \leq \nu < \infty$ .
- (2) The  $\theta$ -chain has eigenvalues  $\lambda_{\nu} = \eta_{\nu} \mu_{\nu}$  with eigenvectors  $q_{\nu}$ ,  $0 \leq \nu < \infty$  and eigenvalues 0 with eigenvectors  $q_{\nu}$  for  $k \leq \nu < \infty$ .
- (3) The random scan chain has spectral decomposition given by eigenvalues  $\frac{1}{2} \pm \frac{1}{2} \sqrt{\eta_{\nu} \mu_{\nu}}$  and eigenvectors  $p_{\nu}(x) \pm \sqrt{\frac{\eta_{\nu}}{\mu_{\nu}}} q_{\nu}(\theta)$  for  $0 \leq \nu < k$  and eigenvalues  $\frac{1}{2}$  and eigenvectors  $q_{\nu}$  for  $k \leq \nu < \infty$ .

**Lemma 17.6.**

$$\mathbb{E}_{\theta} [p_{\nu}(X)] = \eta_{\nu} q_{\nu}(\theta), \quad 0 \leq \nu < k.$$

**Proof.** (1) For  $\nu = 0$ ,  $\mathbb{E}_{\theta} [p_{\nu}] = 1 = \eta_0 q_0$ .

(2) If  $0 < \nu < k$ , then for  $0 \leq i < \nu$  the unconditional expectation is given by

$$\mathbb{E} [\theta^i p_{\nu}(X)] = \mathbb{E} [p_{\nu}(X) \mathbb{E}_X [\theta^i]] = \mathbb{E} [p_{\nu}(X) \hat{p}(X)]$$

with  $\hat{p}$  a polynomial of degree  $i < k$ . Since  $0 \leq i < \nu < k$ ,

$$\mathbb{E} [p_{\nu}(X) \hat{p}(X)] = 0$$

by orthogonality.

(3) Thus,  $0 = \mathbb{E} [\theta^i p_{\nu}(X)] = \mathbb{E} [\theta^i \mathbb{E}_{\theta} [p_{\nu}(X)]]$ .

(4) By assumption (H2)  $\eta_{\nu}^{-1} \mathbb{E}_{\theta} [p_{\nu}(X)]$  is a monic polynomial of degree  $k$  in  $\theta$ .

(5) Since it is orthogonal to all polynomials of degree less than  $k$ ,

$$\mathbb{E}_{\theta} [p_{\nu}(X)] = \eta_{\nu} q_{\nu}(\theta).$$

□

**Lemma 17.7.**

$$\mathbb{E}_x [q_\nu(\theta)] = \mu_\nu p_\nu(x), \quad 0 \leq \nu < k.$$

If  $k < \infty$ ,  $\mathbb{E}_x [q_\nu(\theta)] = 0$  for  $\nu \geq k$ .

**Proof.** (1) The first part is proved as in 17.6.

(2) If  $k < \infty$  and  $\nu \geq k$  by the same argument, for  $0 \leq j < c$ ,

$$\mathbb{E} [p_j(X) \mathbb{E}_X [q_\nu(\theta)]] = 0.$$

(3) But  $p_j$ ,  $0 \leq j < k$  form a basis for  $L^2(m(dx))$  and  $\mathbb{E}_X [q_\nu(\theta)] \in L^2(m(dx))$  since

$$\mathbb{E} [(\mathbb{E}_X [q_\nu(\theta)])^2] \leq \mathbb{E} [q_\nu^2(\theta)] < \infty.$$

(4) Then  $\mathbb{E}_X [q_\nu(\theta)] = 0$  follows. □

**Proof.** (1) Suppose  $0 \leq \nu < k$ . From the definitions, the  $x$ -chain operates on  $p_\nu$  as

$$\mathbb{E}_x [\mathbb{E}_\theta [p_\nu(X')]] = \mathbb{E}_x [\eta_\nu q_\nu(\theta)] = \eta_\nu \mu_\nu p_\nu(x)$$

with equalities from Lemma 17.6 and Lemma 17.7. This proves part 1.

(2) Suppose  $0 \leq \nu < k$ . Then as in the previous step, the  $\theta$ -chain operates on  $q_\nu$  as

$$\mathbb{E}_\theta [\mathbb{E}_x [q_\nu(\theta')]] = \mathbb{E}_\theta [\mu_\nu p_\nu(\theta)] = \mu_\nu \eta_\nu q_\nu(x)$$

with equalities from Lemma 17.6 and Lemma 17.7. This proves part 2. If  $k < \infty$ , then for  $\nu \geq k$ , Lemma 17.7 shows that  $q_\nu$  is an eigenfunction for the  $\theta$ -chain with eigenvalue 0.

(3) The random scan chain takes  $L^2(P)$  into  $L^2(m) + L^2(\pi) \subseteq L^2(P)$ . Then  $\ker K \supseteq L^2(m) + L^2(\pi)^\perp$ . Then

$$Kg(X, \theta) = \frac{1}{2} \mathbb{E}_x [g(x, \theta')] + \frac{1}{2} \mathbb{E}_\theta [g(X', \theta)].$$

(4) For  $0 \leq \nu < k$ , consider  $K$  acting on  $p_\nu(x) + \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta)$ . The result is

$$\begin{aligned} \frac{1}{2} \left( p_\nu(x) + \sqrt{\frac{\eta_\nu}{\mu_\nu}} \mathbb{E}_x [q_\nu(\theta')] \right) + \frac{1}{2} \left( \mathbb{E}_\theta [p_\nu(x)] + \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \right) \\ = \left( \frac{1}{2} + \frac{1}{2} \sqrt{\eta_\nu \mu_\nu} \right) \left( p_\nu(x) + \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \right). \end{aligned}$$

(5) Similarly, consider  $K$  acting on  $p_\nu(x) - \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta)$

$$\begin{aligned} \frac{1}{2} \left( p_\nu(x) - \sqrt{\frac{\eta_\nu}{\mu_\nu}} \mathbb{E}_x [q_\nu(\theta')] \right) - \frac{1}{2} \left( \mathbb{E}_\theta [p_\nu(x)] - \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \right) \\ = \left( \frac{1}{2} - \frac{1}{2} \sqrt{\eta_\nu \mu_\nu} \right) \left( p_\nu(x) - \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \right). \end{aligned}$$

(6) Suppose first that  $k < \infty$ . For  $\nu \geq k$ , Lemma 17.7 shows  $\mathbb{E}_x [q_\nu(\theta)] = 0$  for all  $x$ . Thus  $Kq_\nu(x, \theta) = \frac{1}{2} q_\nu(\theta)$ .

(7) Further

$$\begin{aligned} & \text{span} \left\{ p_\nu(x) \pm \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \text{ for } 0 \leq \nu < c, \text{ and } q_\nu(\theta) \text{ for } c \leq \nu < \infty \right\} \\ &= \text{span} \{ p_\nu(x) \text{ for } 0 \leq \nu < c, \text{ and } q_\nu(\theta) \text{ for } 0 \leq \nu < \infty \} \\ &= L^2(m) + L^2(\pi). \end{aligned}$$

(8) It follows that  $K$  is diagonalizable with eigenvalues and respective eigenvectors

$$\begin{aligned} \frac{1}{2} \pm \frac{1}{2} \sqrt{\eta_\nu \mu_\nu} & \quad p_\nu(x) \pm \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \quad 0 \leq \nu < c \\ \frac{1}{2} & \quad q_\nu(\theta) \quad c \leq \nu < \infty \end{aligned}$$

and  $Kg = 0$  for  $g \in (L^2(m) + L^2(\pi))^\perp$ .

(9) Suppose next that  $k = \infty$ , then  $K$  is diagonalizable with eigenvalues and respective eigenvectors

$$\frac{1}{2} \pm \frac{1}{2} \sqrt{\eta_\nu \mu_\nu} \quad p_\nu(x) \pm \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta)$$

for  $0 \leq \nu < k$ .

(10) Again

$$\begin{aligned} & \text{span} \left\{ p_\nu(x) \pm \sqrt{\frac{\eta_\nu}{\mu_\nu}} q_\nu(\theta) \right\} \text{ for } 0 \leq \nu < k \\ &= \text{span} \{ p_\nu(x) \text{ for } 0 \leq \nu < c, \text{ and } q_\nu(\theta) \text{ for } 0 \leq \nu < k \} \\ &= L^2(m) + L^2(\pi) \end{aligned}$$

and  $Kg = 0$  for  $g \in (L^2(m) + L^2(\pi))^\perp$ .

□

**Beta/Binomial.** The following is a fairly simple and specific example of applying the convergence results to a common probability situation.

Consider  $(\mathcal{X}, \mathcal{F}) = (\{0 : n\}, 2^{\{0:n\}})$  (where  $\{0 : n\} = \{0, 1, 2, \dots, n\}$  and  $2^{\{0:n\}}$  is the power set of  $\{0 : n\}$ , a finite  $\sigma$ -algebra of sets) as the measure space equipped with the counting measure  $\mu(dx)$ . Consider the family of  $\sigma$ -finite measures defined by the Binomial mass function

$$f_\theta(x) = f(x; \theta) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}$$

for natural number  $x \in \{0 : n\}$ ,  $\theta \in (0, 1)$ .

Consider  $(\Theta, \mathcal{G}) = ((0, 1), \mathcal{B})$  (where  $\mathcal{B}$  is the  $\sigma$ -algebra of Borel sets on  $(0, 1)$ ) as the measure space. Take the *prior distribution* for  $\theta$  as the uniform probability density on  $(0, 1)$ . This is a special case of the Beta distribution with shape parameters  $\alpha = 1$  and  $\lambda = 1$ . The special case will make the example easier by mostly avoiding the technicalities of the Beta distribution without losing much generality.

Together these densities define the bivariate Beta/Binomial density (uniform prior)

$$f(x, \theta) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}.$$

The goal is to sample the marginal distribution  $f(x)$  on  $\mathcal{X}$  using the Gibbs sampler  $x$ -chain. The marginal density,

$$\begin{aligned} m(x) &= \int_0^1 f(x, \theta) \, d\theta \\ &= \frac{n!}{x! \cdot (n-x)!} \int_0^1 \theta^x (1 - \theta)^{n-x} \, d\theta \\ &= \frac{n!}{x! \cdot (n-x)!} \frac{\Gamma(x+1) \cdot \Gamma(n-x+1)}{\Gamma(n+2)} \\ &= \frac{n!}{x!(n-x)!} \frac{x! \cdot (n-x)!}{(n+1)!} \\ &= \frac{1}{n+1}, \end{aligned}$$

the uniform density on  $\{0 : n\}$ , is simple and explicit. As such, characteristics of the marginal density need not be generated by the Gibbs sampler. However, this simple example is ideal for illustrative purposes.

The posterior density with respect to  $\pi(d\theta)$  is

$$\pi(\theta \mid x) = \binom{n}{x} \theta^x (1 - \theta)^{n-x} = \text{Beta}(x+1, n-x+1),$$

a well-known statistical distribution. This means the  $x$ -chain sampler can proceed as

- (1) Given  $x$ , draw  $\theta'$  from  $\text{Beta}(x+1, n-x+1)$ ,
- (2) Then given  $\theta'$ , draw  $x'$  from  $\text{Binomial}(n, \theta')$ .

The transition kernel for the  $x$ -chain is

$$k(x, x') = \int_0^1 \pi(\theta \mid x) f_\theta(x') \pi(d\theta) = \int_{\Theta} \frac{f_\theta(x) \cdot f_\theta(x')}{m(x)} \pi(d\theta).$$

Note further that  $m(x)k(x, x') = m(x')k(x', x)$  so that the  $x$ -chain is reversible with  $m(dx)$  as a stationary distribution. Explicitly, the transition kernel is

$$\begin{aligned}
 k(x, x') &= \int_{\Theta} \frac{f_{\theta}(x) \cdot f_{\theta}(x')}{m(x)} \pi(d\theta) \\
 &= \int_0^1 f_{\theta}(x') \pi(d\theta) \, d\theta \\
 &= \int_0^1 \binom{n}{x} \theta^x (1-\theta)^{n-x} \cdot \binom{n}{x'} \theta^{x'} (1-\theta)^{n-x'} \cdot \frac{1}{1/(n+1)} \, d\theta \\
 &= (n+1) \binom{n}{x} \binom{n}{x'} \int_0^1 \theta^{x+x'} (1-\theta)^{2n-x-x'} \, d\theta \\
 &= (n+1) \binom{n}{x} \binom{n}{x'} \frac{\Gamma(x+x'+1) \Gamma(2n-x-x'+1)}{\Gamma(2n+1)} \\
 &= (n+1) \binom{n}{x} \binom{n}{x'} \frac{(x+x')! (2n-x-x')!}{(2n+1)!} \\
 &= \frac{(n+1)}{2n+1} \frac{\binom{n}{x} \binom{n}{x'}}{\binom{2n}{x+x'}}.
 \end{aligned}$$

This expresses the  $x$ -chain kernel explicitly as a transition probability matrix. Remember that the intention is to use the Gibbs sampler as a simple way to simulate the marginal instead of this direct and explicit calculation.

**Proposition 17.8.** (1) *The  $x$ -chain for the marginal of the Beta/Binomial (uniform prior) has eigenvalues*

$$\begin{aligned}
 \lambda_0 &= 1, \\
 \lambda_j &= \frac{n(n-1) \cdots (n-j+1)}{(n+2)(n+3) \cdots (n+j+1)}, \quad 1 \leq j \leq n.
 \end{aligned}$$

(2) *In particular,  $\lambda_1 = 1 - 2/(n+2)$ .*

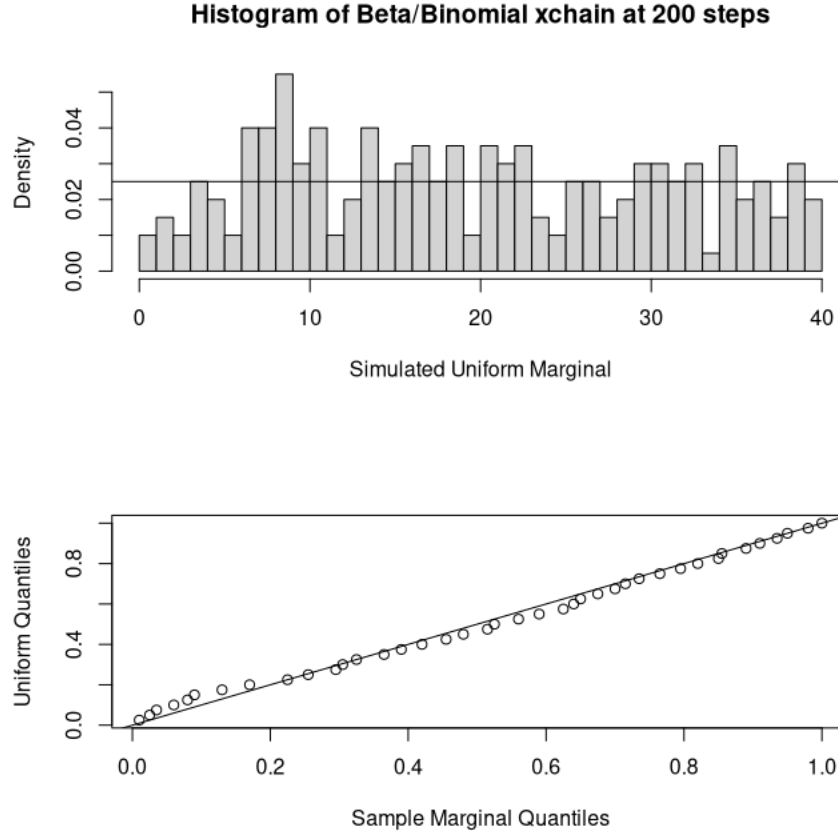
(3) *The eigenfunctions are the orthogonal polynomials for  $m(x) = 1/(n+1)$  on  $\{0 : n\}$ , known as the discrete Chebyshev polynomials.*

**Proof.** Apply previous theorems. □

A script implementing the  $x$ -chain for the Beta/Binomial is in the Scripts section. The results are in Figure 17.1. A script comparing the eigenvalues computed from the transition probability matrix with the theoretical eigenvalues in the Proposition is in the Scripts section. The two sets of values agree to essentially machine precision.

**Poisson/Gamma.** The following example of the  $x$ -chain for the Poisson/Gamma distributions is a generalization of the previous example of the Poisson/Exponential distributions.

Consider  $(\mathcal{X}, \mathcal{F}) = (\mathbb{N}, 2^{\mathbb{N}})$  (where  $2^{\mathbb{N}}$  is the power set of  $\mathbb{N}$ , a  $\sigma$ -algebra of sets) as the measure space equipped with the counting measure  $\mu(dx)$ . Consider the family of  $\sigma$ -finite measures defined by the Poisson mass function  $f_{\theta}(x) = f(x; \theta) = e^{-\theta} \theta^x / x!$  for natural number  $x \in \mathbb{N}$  and parameter  $\theta \in (0, \infty)$ . The usual notation



**Figure 17.1.** Sampling the discrete uniform marginal distribution from the Beta/Binomial with uniform prior. The QQ plot demonstrates good agreement of the sample quantiles with the discrete uniform distribution. Agreement with the discrete uniform mass function is harder to see in the histogram.

for the Poisson mass function parameter is  $\lambda$  but this example uses  $\theta$  to be consistent with the section on Two-Component Gibbs Sampling.

Consider  $(\Theta, \mathcal{G}) = ((0, \infty), \mathcal{B})$  (where  $\mathcal{B}$  is the  $\sigma$ -algebra of Borel sets on  $(0, \infty)$ ) as the measure space. Fix parameters  $\alpha$  and  $a > 0$  for the Gamma function. Take the *prior distribution* as the Gamma probability density with shape parameter  $a$  and scale parameter  $\alpha$

$$\pi(\theta; a, \alpha) = \frac{\theta^{a-1} e^{-\theta/\alpha}}{\alpha^a \Gamma(a)}$$

as a family of probability densities on  $(0, \infty)$  with respect to Lebesgue measure. When  $\alpha = 1$  and  $a = 1$ , the prior is the exponential density  $e^{-\theta}$ , as in the previous example of the Poisson/Exponential chain.

Following the derivation in the section on Two-Component Gibbs Sampling the marginal density on  $\mathcal{X} = \mathbb{N}$  is

$$\begin{aligned}
 m(x) &= \int_{\Theta} f_{\theta}(x) \pi(d\theta) = \int_0^{\infty} \frac{e^{-\theta} \theta^x}{x!} \cdot \frac{\theta^{a-1} e^{-\theta/\alpha}}{\alpha^a \Gamma(a)} d\theta \\
 &= \frac{1}{\alpha^a \Gamma(a) x!} \int_0^{\infty} e^{-(1+1/\alpha)\theta} \theta^{x+a-1} d\theta \\
 &= \frac{1}{\alpha^a \Gamma(a) x!} \frac{1}{((\alpha+1)/\alpha)^{x+a-1}} \frac{1}{((\alpha+1)/\alpha)} \cdot \\
 &\quad \int_0^{\infty} e^{-((\alpha+1)/\alpha)\theta} \left(\frac{\alpha+1}{\alpha}\theta\right)^{x+a-1} d\left(\frac{\alpha+1}{\alpha}\theta\right) \\
 &= \frac{1}{\alpha^a \Gamma(a) x!} \frac{1}{((\alpha+1)/\alpha)^{x+a}} \int_0^{\infty} e^{-z} z^{x+a-1} dz \\
 &= \frac{1}{\alpha^a \Gamma(a) x!} \frac{\Gamma(x+a)}{((\alpha+1)/\alpha)^{x+a}} \\
 &= \frac{\alpha^x}{x! (\alpha+1)^{x+a}} \frac{\Gamma(x+a)}{\Gamma(a)} \\
 &= \frac{(a)_x}{x!} \left(\frac{1}{\alpha+1}\right)^a \left(\frac{\alpha}{\alpha+1}\right)^x.
 \end{aligned}$$

The last equality follows from the Gamma function identities

$$\Gamma(a+x) = a(a+1)(a+2) \cdots (a+x-1)\Gamma(a) = (a)_x \Gamma(a)$$

where  $(a)_x$  is the rising Pochhammer symbol, also called the shifted factorial,

$$(a)_x = \begin{cases} 1 & x = 0, \\ a(a+1)(a+2) \cdots (a+x-1) & x > 0. \end{cases}$$

See the exercises for a direct proof that the marginal distribution is a probability distribution.

When  $a$  is a positive integer,

$$m(x) = \frac{(a)_x}{x!} \left(\frac{1}{\alpha+1}\right)^a \left(\frac{\alpha}{\alpha+1}\right)^x$$

is the negative binomial distribution for the additional number  $x$  of independent Bernoulli trials, i.e. failures, required to attain  $a$  successes, each with success probability  $1/(\alpha+1)$ . In that case the term

$$\frac{(a)_n}{x!} = \frac{a(a+1)(a+2) \cdots (a+x-1)}{x!} = \binom{a+x-1}{a-1}$$

is the usual expression in the negative binomial distribution. The calculation of the marginal distribution is the derivation of the negative binomial as a continuous mixture of Poisson distributions where the mixing distribution of the Poisson rate is a Gamma distribution. In the special case of the Poisson/Exponential example where  $\alpha = a = 1$ , the general form of the marginal reduces to  $m(x) = 1/2^{x+1}$ .

The posterior density with respect to  $\pi(d\theta)$  is

$$\begin{aligned}\pi(\theta | x) &= f_\theta(x)/m(x) = f(x; \theta)/m(x) \\ &= \frac{e^{-\theta} \theta^x}{x!} \cdot \frac{x!}{\alpha^x} \cdot \frac{\Gamma(a)(\alpha+1)^{x+a}}{\Gamma(x+a)} \\ &= \frac{e^{-\theta} \theta^x \Gamma(a) \alpha^a}{\Gamma(x+a)} \left( \frac{\alpha+1}{\alpha} \right)^{x+a} \\ &= \frac{e^{-\theta} \theta^x (\alpha+1)^{x+a}}{\alpha^x (a)_x}.\end{aligned}$$

The  **$x$ -chain** is: first draw  $\theta'$  from  $\pi(\theta' | x)$  and then  $x'$  from  $f_{\theta'}(x')$ . The  $x$ -chain has transition kernel

$$\begin{aligned}k(x, x') &= \int_0^\infty \pi(\theta | x) f_\theta(x') \pi(d\theta) \\ &= \int_0^\infty \frac{e^{-\theta} \theta^x \Gamma(a) \alpha^a}{\Gamma(x+a)} \left( \frac{\alpha+1}{\alpha} \right)^{x+a} \cdot \frac{e^{-\theta} \theta^{x'}}{x'!} \cdot \frac{\theta^{a-1} e^{-\theta/\alpha}}{\Gamma(a) \alpha^a} d\theta \\ &= \int_0^\infty \frac{e^{-(1+1/\alpha)\theta} \theta^{x+a-1}}{\Gamma(x+a) (\alpha/(\alpha+1))^{x+a}} \cdot \frac{e^{-\theta} \theta^{x'}}{x'!} d\theta \\ &= \frac{1}{\Gamma(x+a) (\alpha/(\alpha+1))^{x+a}} \frac{1}{x'!} \int_0^\infty e^{-(2+1/\alpha)\theta} \theta^{x+x'+a-1} d\theta \\ &= \frac{\Gamma(x+x'+a) (\alpha/(2\alpha+1))^{x+x'+a}}{\Gamma(x+a) (\alpha/(\alpha+1))^{x+a} x'!}.\end{aligned}$$

The last integral follows from the definition of the gamma function, see the exercises

When  $\alpha = a = 1$ , the prior is the negative binomial probability distribution and the transition kernel reduces to

$$\begin{aligned}k(x, x') &= \binom{x+x'}{x} \left( \frac{1}{3} \right)^{x+x'+1} / \left( \frac{1}{2} \right)^{x+1}, \\ m(x) &= 1/2^{x+1}.\end{aligned}$$

The Gauss series defines the regular hypergeometric function

$$\begin{aligned}{}_2F_1(a, b; c; z) &= 1 + \frac{a \cdot b}{c} \frac{z}{1!} + \frac{a(a+1) \cdot b(b+1)}{c(c+1)} \frac{z^2}{2!} + \dots \\ &= \sum_{\nu=0}^{\infty} \frac{(a)_\nu (b)_\nu}{(c)_\nu} \frac{z^\nu}{\nu!}\end{aligned}$$

which converges (if  $c \neq 0, -1, -2, \dots$ ) for  $|z| < 1$ . If  $a = 0, -1, -2, \dots$  is a negative integer, the regular hypergeometric function is a degree  $-a$  polynomial.

The orthogonal polynomials for the negative binomial are Meixner polynomials  $M_j(x; a, \alpha)$ . See the exercises. The Meixner polynomials (also called discrete Laguerre polynomials) are a family of discrete orthogonal polynomials on  $\mathcal{X} = \{0, 1, 2, 3, \dots\}$  introduced by Josef Meixner in 1934. One definition of the Meixner polynomials in terms of the regular hypergeometric function is

$$M_j(x; a, \alpha) = {}_2F_1(-j, -x; a; -\alpha).$$



In this definition, the parameter  $\alpha > 0$  corresponds to a Bernoulli trial success probability  $\frac{1}{\alpha+1}$  and the integer parameter  $a$  corresponds to the number of successes in the negative binomial distribution. An alternate definition [Chi78, V-3.4, page 161] with a different normalization is

$$m_j(x; \beta, c) = (\beta)_j \cdot {}_2F_1(-j, -x; \beta; 1 - 1/c).$$

where  $0 < c < 1$  and  $\beta > 0$ . In the second alternative normalized definition for  $m_j$  the parameter  $c$  represents the success probability  $1/(\alpha+1)$  so  $-\alpha = 1 - 1/c$ . With the correspondence  $\beta = a$  and  $c = 1/(\alpha+1)$

$$m_j(x; a, 1/(\alpha+1)) = (a)_j M_j(x; a, \alpha).$$

The following discussion will use  $M_j(x; a, \alpha)$  as the definition of the Meixner polynomials.

The first three Meixner polynomials are

$$\begin{aligned} M_0(x; a, \alpha) &= 1, \\ M_1(x; a, \alpha) &= 1 - \frac{\alpha}{a}x = \frac{a - \alpha x}{a}, \\ M_2(x; a, \alpha) &= 1 - \frac{2\alpha}{a}x + \frac{\alpha^2}{a(a+1)}x(x+1). \end{aligned}$$

See the exercises.

The orthogonality relation for the normalized Meixner polynomials, see [Chi78, VI-3.4, 176], slightly rewritten here to emphasize the negative binomial weight function and using the parameter correspondence, is

$$\sum_{x=0}^{\infty} m_j(x; a, \alpha) m_\ell(x; a, \alpha) \frac{(a)_x}{x!} \left( \frac{1}{\alpha+1} \right)^x \left( \frac{\alpha}{\alpha+1} \right)^a = \left( \frac{1}{\alpha+1} \right)^{-j} j! (a)_j \delta_{j\ell}.$$

This can be verified from the generating function definition of the Meixner polynomials, see the exercises. Dividing through by  $(a)_j$  and  $(a)_\ell$  and rearranging slightly (and simplifying by using  $(a)_\ell = (a)_j$  when  $j = \ell$ ), now the orthogonality relation for the unnormalized Meixner polynomials is

$$\sum_{x=0}^{\infty} M_j(x) M_\ell(x) m(x) = \frac{(1+\alpha)^j j!}{(a)_j} \delta_{j\ell}.$$

In Section 18.19, the Digital Library of Mathematical Functions gives the formula for the leading coefficients of the Meixner polynomials as

$$M_n(x; \beta, c) = (1 - 1/c)^n / (\beta)_n.$$

Note the falling Pochhammer symbol. In Section 18.19, the Digital Library of Mathematical Functions also gives the expression for the orthogonality conditions. [ But the symbols need to be unraveled.]

**Proposition 17.9.** *For  $a > 0$ ,  $\alpha > 0$  the Poisson/Gamma  $x$ -chain has*

- (1) *Eigenvalues  $\lambda_j = (\alpha/(1+\alpha))^j$ , for  $0 \leq j < \infty$ ,*
- (2) *Eigenfunctions  $M_j(x)$ , the Meixner polynomials,*

(3) For any  $\ell \geq 0$  and any starting state  $x$

$$\chi_x^2(\ell) = \sum_{y=0}^{\infty} \frac{(k^\ell(x, y) - m(y))^2}{m(y)} = \sum_{\nu=1}^{\infty} \lambda_\nu^{2\ell} M_\nu^2(x) \frac{(a)_\nu}{(1+\alpha)^\nu \nu!}.$$

**Corollary 17.10.** For  $\alpha = a = 1$ , starting at  $n$ ,

$$\begin{aligned} \chi_n^2(\ell) &\leq 2^{-2c} & \ell = \log_2(n+1) + c, c > 0 \\ \chi_n^2(\ell) &\geq 2^{2c} & \ell = \log_2(n-1) - c, c > 0. \end{aligned}$$

**Proof.** (1) From the definitions, for all  $j$  and positive integers  $x$ , using the Triangle Inequality

$$\begin{aligned} |M_j(x)| &= \left| \sum_{\nu=0}^{\min(j,x)} (-1)^\nu \binom{j}{\nu} x(x-1) \cdots (x-\nu+1) \right| \\ &\leq \sum_{\nu=0}^j \binom{j}{\nu} x^\nu = (1+x)^j. \end{aligned}$$

(2) Thus, for  $\ell \geq \log_2(1+n) + c$ ,

$$\begin{aligned} \chi_n^2(\ell) &= \sum_{\nu=1}^{\infty} M_\nu^2(n) 2^{-\nu(2\ell+1)} \leq \sum_{\nu=1}^{\infty} (1+n)^{2j} 2^{-\nu(2\ell+1)} \\ &\leq \frac{(1+n)^2 2^{-(2\ell+1)}}{1 - (1+n)^2 2^{-(2\ell+1)}} \leq \frac{2^{-2c-1}}{1 - 2^{-2c-1}} \leq 2^{-2c}. \end{aligned}$$

(3) The lower bound follows from using only the lead term, namely

$$\chi_n^2(\ell) \geq (1-n)^2 2^{-2\ell} \geq 2^{2c}$$

for  $\ell = \log_2(n-1) - c$ .

□

## 17.5. Birth and Immigration Example

A simple model of population dynamics with immigration is a Markov chain. For this birth and immigration Markov chain the state space is  $\mathcal{X} = \{0, 1, 2, \dots\}$ . If the population size at generation  $n$  is  $X_n$ , then given  $X_n = x$ ,

$$X_{n+1} = \sum_{\nu=1}^x N_{\nu,n} + M_{n+1}$$

where  $N_{\nu,n}$  is the random number of offspring of member  $\nu$  of the population at time  $n$ . The offspring random variables  $N_{\nu,n}$  are independent, and identically distributed geometric random variables with parameter  $\frac{1}{3}$ , that is

$$\mathbb{P}[N_{\nu,n} = j] = \frac{2}{3} \left(\frac{1}{3}\right)^j, 0 \leq j < \infty.$$

Assume the random variable  $M_{n+1}$  is immigration with the same distribution as  $N_{\nu,n}$  and independent of  $N_{\nu,n}$ . Suppose the population is  $x$ . The sum of  $x+1$

independent, identically distributed geometric random variables with parameter  $p$  being exactly value  $y$  has a negative binomial distribution,

$$p(x, y) = \binom{x+1+y-1}{x} \left(\frac{1}{3}\right)^{x+1} \left(\frac{2}{3}\right)^y.$$

Taking the reference measure as counting measure, and the probability measure as  $m(x) = \frac{1}{2^{x+1}}$  the transition probability can be written as

$$(17.2) \quad p(x, y) = \left(\frac{1}{3}\right)^{x+y+1} \binom{x+y}{x} / \left(\frac{1}{2}\right)^{x+1}.$$

Note that by the symmetry of  $x$  and  $y$  in the transition probability kernel, the Markov chain is reversible. From (17.2) the eigenvalues are  $\lambda_j = \frac{1}{2^j}$  for  $j = 0, 1, 2, \dots$ . The eigenfunctions are the orthogonal polynomials for the measure  $\mu(x) = \frac{1}{2^{x+1}}$ . These are the Meixner polynomials.

Now applying the spectral representation with Corollary 17.10, for any starting state  $x$  for all  $n \geq 0$

$$\chi_x^2(n) = \sum_{y=0}^{\infty} \frac{(p^n(x, y) - m(y))^2}{m(y)} = \sum_{\nu=1}^{\infty} \lambda_{\nu}^{2n} M_{\nu}^2(x) \frac{1}{2^{\nu}}.$$

This gives bounds on the convergence. With the notation of Corollary 17.10,

$$\begin{aligned} \chi_x^2(n) &\leq 2^{-2c} \text{ for } n = \log_2(x+1) + c, c > 0 \\ \chi_x^2(n) &\geq 2^{2c} \text{ for } n = \log_2(x-1) + c, c > 0. \end{aligned}$$

The results show the convergence is rapid, only order  $\log_2(x)$  steps are necessary and sufficient for convergence to stationarity.

## 17.6. Chapter Ending Answer

Label the states conveniently as  $(R, N, S) = (x_1, x_2, x_3)$  so the Rain starting state is  $(1, 0, 0)$ . The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} R & N & S \end{matrix} \\ \begin{matrix} R \\ N \\ S \end{matrix} & \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix} \end{matrix}.$$

The eigenvalues of  $P$  are  $1, 1/4, -1/4$  with corresponding normalized left eigenvectors

$$(2/3, 1/3, 2/3), (1/\sqrt{2}, 0, -1/\sqrt{2}), (1/\sqrt{6}, -2/\sqrt{6}, 1/\sqrt{6}).$$

Using unnormalized left eigenvectors with rational entries, and expressing the starting state in terms of these eigenvectors  $(1, 0, 0) = (1/2) \cdot (1, 0, -1) + (1/10) \cdot (1, -2, 1) + (2/5) \cdot (1, 1/2, 1)$ . Note that  $(2/5) \cdot (1, 1/2, 1)$  is the stationary distribution. Then the state at time  $n$  is

$$\begin{aligned} (1, 0, 0)P^n &= \\ &= (1/4)^n \cdot (1/2) \cdot (1, 0, -1) + (-1/4)^n \cdot (1/10) \cdot (1, -2, 1) + (1)^n \cdot (2/5) \cdot (2, 1, 2). \end{aligned}$$

Then the Euclidean distance from the stationary distribution is

$$D = \sqrt{\left[\frac{1}{2} \left(\frac{1}{4}\right)^n + \frac{1}{10} \left(\frac{-1}{4}\right)^n\right]^2 + \left[\frac{-1}{5} \left(\frac{1}{4}\right)^n\right]^2 + \left[\frac{-1}{2} \left(\frac{1}{4}\right)^n + \frac{1}{10} \left(\frac{-1}{4}\right)^n\right]^2} \\ = \sqrt{\frac{14}{25} \left(\frac{1}{16}\right)^n} = \frac{\sqrt{14}}{5} \left(\frac{1}{4}\right)^n.$$

This example does not fit precisely in the framework of this section since  $P$  is not self-adjoint. However, it does illustrate the precise bounds that can be achieved if the eigenvalue and eigenvectors are known.

## 17.7. Chapter Summary

### Key Concepts.

- (1) The **systematic scan Gibbs sampler** for drawing from the distribution  $\mathbb{P}[\cdot]$  proceeds as follows. Starting from  $(x, \theta)$ , first, draw  $x'$  from  $f_\theta(\cdot)$ ; second, draw  $\theta'$  from  $\pi(\cdot | x')$ . The output is  $(x', \theta')$ . This generates a Markov chain  $(x, \theta) \rightarrow (x', \theta') \rightarrow \dots$  having kernel

$$K(x, \theta; x', \theta') = f_\theta(x') \cdot f_{\theta'}(x') / m(x')$$

with respect to  $\mu(dx')\pi(d\theta)$ .

- (2) The  **$x$ -chain** is: first, draw  $\theta'$  with probability  $\pi(\theta' | x)$ ; second,  $x'$  with probability  $f_{\theta'}(x')$  (with the abuse of notation that the probability is given by the density function  $f_{\theta'}(x')$ ). The  $x$ -chain has transition kernel

$$k(x, x') = \int_{\Theta} \pi(\theta | x) f_\theta(x') \pi(d\theta) = \int_{\Theta} \frac{f_\theta(x) \cdot f_\theta(x')}{m(x)} \pi(d\theta).$$

- (3) The  **$\theta$ -chain** is: first draw  $x$  from  $f_\theta(x)$  and then  $\theta'$  from  $\pi(\theta' | x)$ . The  $\theta$ -chain has transition kernel

$$k(\theta, \theta') = \int_{\mathcal{X}} f_\theta(x) \pi(\theta' | x) \mu(dx) = \int_{\mathcal{X}} \frac{f_\theta(x) f_{\theta'}(x)}{m(x)} \mu(dx).$$

- (4) Under simple hypotheses common Gibbs sampler Markov chains have polynomial eigenvectors, with explicitly known eigenvalues. This includes the  $x$ -chain,  $\theta$ -chain and the random scan chain.
- (5) An example of the  $x$ -chain for the Poisson/Gamma distributions gives explicit expressions for the eigenvalues and eigenvectors in terms of the orthogonal polynomial system of Meixner polynomials.
- (6) A simple model of population dynamics with immigration is a Markov chain. The results show the convergence is rapid, only order  $\log_2(x)$  steps are necessary and sufficient for convergence to stationarity.

### Vocabulary.

- (1) The **systematic scan Gibbs sampler** for drawing from the distribution  $\mathbb{P}[\cdot]$  proceeds as follows. Starting from  $(x, \theta)$ , first, draw  $x'$  from  $f_\theta(\cdot)$ ; second, draw  $\theta'$  from  $\pi(\cdot | x')$ .

- (2) For the joint density  $f(x, \theta)$  the  **$x$ -chain** is the Markov chain created by the process: From  $x$ , draw  $\theta'$ , from  $\pi(\theta' | x)$  and then  $x'$  from  $f_{\theta'}(x')$
- (3) The  **$\theta$ -chain** is: first draw  $x$  from  $f_{\theta}(x)$  and then  $\theta'$  from  $\pi(\theta' | x)$ .
- (4) The **random scan chain** proceeds as follows. From  $(x, \theta)$ , pick a coordinate at random equally, and update it from the appropriate conditional distribution. Then formally, for  $g \in L^2(\mathbb{P})$

$$\bar{K}g(x, \theta) = \frac{1}{2} \int_{\Theta} g(x, \theta'') \pi(\theta'' | x) \pi(d\theta'') + \frac{1}{2} \int_{\mathcal{X}} g(x', \theta) f_{\theta}(x') \mu(dx').$$

- (5) The **chi-square distance** between the distribution of the chain started at  $\xi$  after  $\ell$  steps and its stationary measure is

$$\chi_{\xi}^2(\ell) = \int \left| \hat{K}_{\xi}^{\ell}(\xi') - 1 \right|^2 m(d\xi') = \int \frac{|K^{\ell}(\ell, \ell') - m(\xi')|^2}{m(\xi')} \mu(d\xi').$$

#### Notation.

- (1)  $\mathcal{X}$  – state space, either finite or infinite
- (2)  $\mu(dx)$  – reference measure on  $\mathcal{X}$ ,
- (3)  $m(x)$  – a probability density with respect to  $\mu$ ,
- (4)  $P(x, dy)$  – for each  $x$ ,  $P(x, \cdot)$  is a probability measure on  $\mathcal{X}$ .
- (5)  $X_0, X_1, X_2, \dots$  – a Markov chain with starting state  $X_0 = x$
- (6)  $f, g$  – square integrable functions with respect to  $m$
- (7)  $P(x, dy) = p(x, y) \mu(dy)$  – density form of the kernel
- (8)  $\lambda_{\nu}$  – eigenvalues and corresponding eigenvectors  $f_{\nu}$  so that  $Pf_{\nu} = \lambda_{\nu} f_{\nu}$  for  $\nu = 0, 1, 2, \dots$
- (9)  $(\mathcal{X}, \mathcal{F})$  – measure space for states
- (10)  $\theta$  – parameter for the distribution
- (11)  $(\Theta, \mathcal{G})$  – measure space for priors
- (12)  $\{f_{\theta}(x) : \theta \in \Theta\}$  – family of probability densities on  $\mathcal{X}$  with respect to measure  $\mu(dx)$
- (13)  $A \in \mathcal{F}, B \in \mathcal{G}$  – arbitrary sets
- (14)  $m(x) = \int_{\Theta} f_{\theta}(x) \pi(d\theta)$  – marginal density
- (15)  $\pi(\theta | x) = f_{\theta}(x) / m(x)$  – posterior density with respect to  $\pi(d\theta)$
- (16)  $K(x, \theta; x', \theta')$  – kernel for systematic scan Gibbs sampler starting from  $x$
- (17)  $\tilde{K}(x, \theta; x', \theta')$  – kernel for systematic scan Gibbs sampler starting from  $\theta$
- (18)  $k(x, x')$  – kernel for  $x$ -chain
- (19)  $k(\theta, \theta')$  – kernel for  $\theta$ -chain
- (20)  $\text{bar}Kg(x, \theta)$  – action of random scan chain
- (21)  $I_0(z) = \sum_{\nu=0}^{\infty} \frac{1}{(\nu!)^2} \left(\frac{z}{2}\right)^{2\nu}$  – modified Bessel function of order 0
- (22)  $K(\xi, \xi')$  – general kernel for a Markov chain

- (23)  $\chi_\xi^2(\ell)$  – **chi-square distance** between the distribution of the chain started at  $\xi$  after  $\ell$  steps and its stationary measure
- (24)  $(\mathcal{X}, \mathcal{F}) = (\mathbb{N}, 2^{\mathbb{N}})$  – the measure space equipped with the counting measure  $\mu(dx)$  for the Poisson distribution
- (25)  $\theta$  – parameter for the Poisson distribution
- (26)  $(\Theta, \mathcal{G}) = ((0, \infty), \mathcal{B})$  – the measure space for the Gamma distribution
- (27)  $a$  – shape parameter for the Gamma distribution
- (28)  $\alpha$  – scale parameter for the Gamma distribution
- (29)  $\pi(\theta; a, \alpha) = \frac{\theta^{a-1} e^{-\theta/\alpha}}{\alpha^a \Gamma(a)}$  – family of Gamma probability densities
- (30)  $\text{Gamma}(a)$  – Gamma function
- (31)  $(a)_x$  – the rising Pochhammer symbol, also called the shifted factorial  
item  ${}_2F_1(a, b; c; z)$  – the regular hypergeometric function
- (32)  $M_j(x; a, \alpha) = {}_2F_1(-j, -x; a; -\alpha)$  – the Meixner polynomials in terms of the regular hypergeometric function
- (33)  $m_j(x; \beta, c) = (\beta)_j \cdot {}_2F_1(-j, -x; \beta; 1 - 1/c)$  – alternate definition of Meixner polynomials with a different normalization
- (34)  $\delta_{jk}$  – Kronecker delta function
- (35)  $N_{\nu, n}$  – the random number of offspring of member  $\nu$  of the population at time  $n$
- (36)  $M_{n+1}$  – the immigration with the same distribution as  $N_{\nu, n}$

## 17.8. Sources

This section is adapted from: The Markov Chain Monte Carlo Revolution by Persi Diaconis [Dia09] and Gibbs Sampling, Exponential Families and Orthogonal Polynomials by Diaconis, Khare, and Saloff-Coste [DKSC08].

The negative binomial as a continuous mixture of Poisson distributions where the mixing distribution of the Poisson rate is a Gamma distribution is from NegativeBinomialDistribution.

The definition of the regular hypergeometric function as a Gauss series is from the Digital Library of Mathematical Functions, Section 15.2, Digital Library of Mathematical Functions, Gauss Series

Information about the Meixner polynomials is from Chihara [Chi78].

## 17.9. Algorithms and Scripts

### Algorithm.

### Scripts.

**R:** R script for the BetaBinomial x-chain.

```

1 xchain<-function (x, n) {
2   thetap <- rbeta(1, x+1, n-x+1)
3   xp      <- rbinom(1, n, thetap)

```

**Data:** Size of binomial, length of the  $x$ -chain, starting value for the  $x$ -chain, number of trials

**Result:** Plots of Gibbs sampler results, total variation distance to uniform

```

1 function xchain(x, n)
2   | one step of the  $x$  by selecting  $\theta$  from Beta distribution, then  $x$  from
   | Binomial
3 Set size of binomial  $n$ , length of the  $x$ -chain  $L$ , starting value  $x_0$  for the
    $x$ -chain, number of trials  $r$ 
4 Set recording period and determine number of records
5 Initialize records of the  $x$ -chain and total variation distance
6 for  $x \leftarrow 1 : r$  do
7   | for  $i \leftarrow 1 : L$  do
8   |   |  $x_0 \leftarrow \text{xChain}(x_0, n)$ 
9   |   | Record  $x_0$  at recording periods
10  | end
11 end
12 Compute total distribution distance to uniform at recording periods
13 Plot histogram and QQ plot of results

```

**Data:** Size of binomial

**Result:** Comparison of computed eigenvalues with theoretical eigenvalues

```

1 Set size of binomial  $n$ 
2 Fill transition probability matrix with Pxxp Compute eigenvalue, in
   decreasing order
3 Compute theoretical eigenvalues, in decreasing order
4 Summarize difference of computed and theoretical eigenvalues

```

```

4 }
5
6 n <- 39      #size of binomial, chosen so lambda_1 = 1
              -2/(n+1) = 0.95
7 L <- 200     #length of xchain, chosen so L =
              multiple of n
8 x0 <- n      #starting value for xchain, following
              Diaconis
9 trials <- 200  #number of trials
10
11 p <- 10      # recording period
12 k <- L %/% p  # number of records
13 xrecord <- matrix(NA, nrow=k, ncol=trials)
14 distTV <- numeric(k)
15
16 for (r in 1:trials) {
17   for (i in 1:L) {
18     x0 <- xchain(x0, n)
19     if ( i % p == 0) {

```

```

20         xrecord[ i/p, r ] <- x0
21     }
22 }
23 }
24
25 for (i in 1:k) {
26     xempir <- hist(xrecord[i, ], breaks=0:(n+1),
27         right=FALSE, plot=FALSE)$density
28     distTV[i] <- (1/2) * sum( abs( xempir - 1/(n+1) )
29 )
30 }
31
32 par( mfrow=c( 2, 1 ) )
33 hist(xrecord[ k, ], breaks=0:(n+1),
34     main = paste("Histogram of Beta/Binomial xchain
35 at", L, "steps"),
36     xlab = "Simulated Uniform Marginal",
37     right=FALSE, freq=FALSE)
38 abline( c( 1/(n+1), 0 ) )
39
40 xempir <- hist(xrecord[ k, ], breaks=0:(n+1), right=
41     FALSE, plot=FALSE)$density
42 yunif <- rep( 1/(n+1), n+1 )
43 qqplot( cumsum(xempir), cumsum(yunif),
44     xlab = "Sample Marginal Quantiles", ylab = "
45     Uniform Quantiles",)
46 abline( c(0,1) )

```

R script for eigenvalues of the BetaBinomial x-chain.

```

1 Pxxp <- function(n, x, xp) {
2     ((n+1)/(2*n+1)) * (choose(n,x) * choose(n,xp))/
3     choose(2*n, x+xp)
4 }
5
6 n <- 100
7
8 P <- matrix(NA, nrow=n+1, ncol=n+1)
9
10 for (row in 1:(n+1)) {
11     P[row, ] <- Pxxp(n, row-1, 0:n)
12 }
13
14 evals <- rev(sort( eigen(P)$values))
15
16 lambda <- function(n, j) {

```



```

16      prod( seq(n, n-j+1, by = -1) ) / prod(seq(n+2, n+j
      +1))
17  }
18
19  theorevals <- numeric(n)
20  for (j in 1:n) { theorevals[j] = lambda(n,j) }
21
22  summary( evals[2:(n+1)] - theorevals )

```

### 17.10. Problems to Work for Understanding

1: Show

$$m(x) = \int_0^{\infty} \frac{e^{-\theta} \theta^x}{x!} e^{-\theta} d\theta = \int_0^{\infty} \frac{e^{-2\theta} \theta^x}{x!} d\theta = \frac{1}{2^{x+1}}.$$

2: Show

$$\int_0^{\infty} \frac{2^{x+1} \theta^{x+x'} e^{-3\theta}}{x! x'!} d\theta = \frac{2^{x+1}}{3^{x+x'+1}} \binom{x+x'}{x}, \quad x, x' \in \{0, 1, 2, 3, \dots\}.$$

3: Show

$$\frac{(a)_x}{x!} \left( \frac{1}{\alpha+1} \right)^a \left( \frac{\alpha}{\alpha+1} \right)^x$$

is a probability mass function for  $x = 0, 1, 2, 3, \dots$

4: Show

$$\begin{aligned} k(x, y) &= \int_0^{\infty} \frac{e^{-\text{lambda}(\alpha+1)/\alpha} \text{lambda}^{a+x-1}}{\Gamma(a+x)(\alpha/(\alpha+1))^{a+x}} \cdot \frac{e^{-\text{lambda}} \text{lambda}^y}{y!} d\text{lambda} \\ &= \frac{\Gamma(a+x+y)(\alpha/(2\alpha+1))^{a+x+y}}{\Gamma(a+x)(\alpha/(\alpha+1))^{a+x} y!}. \end{aligned}$$

5: Show the first three Meixner polynomials are

$$\begin{aligned} M_0(x; a, \alpha) &= 1, \\ M_1(x; a, \alpha) &= 1 - \frac{\alpha}{a} x = \frac{a - \alpha x}{a}, \\ M_2(x; a, \alpha) &= 1 - \frac{2\alpha}{a} x + \frac{\alpha^2}{a(a+1)} x(x+1), \end{aligned}$$

6: Verify the orthogonality relation for the Meixner polynomials

$$\sum_{x=0}^{\infty} M_j(x) M_k(x) m(x) = \frac{(1+\alpha)^j j!}{(a)_j} \delta_{jk}$$

for  $j = k = 0$ ;  $j = 0, k = 1$ ; and  $j = k = 1$ .

7: Using Meixner's generating function

$$G(x, w) = \left(1 - \frac{w}{c}\right)^x (1 - w)^{-x-\beta}$$

with  $0 < |c| < 1$  and  $\beta \neq 0, -1, -2, \dots$ , verify the orthogonality condition for the normalized Meixner polynomials

$$\sum_{x=0}^{\infty} m_j(x; \beta, c) m_k(x; \beta, c) \frac{(\beta)_x}{x!} c^x (1 - c)^\beta = c^{-j} j! (\beta)_j \delta_{jk}.$$



## Fastest Mixing Markov Chain

This chapter considers the problem of assigning transition probabilities to the edges+ of a simple linear network in such a way that the resulting Markov chain mixes as rapidly as possible. The problem is equivalent to assigning probabilities to a random walk with partially reflecting boundaries with each step either to the vertex itself or its nearest neighbor. It is also equivalent to certain urn models. The article proves the fastest mixing is obtained when each edge has a transition probability of  $1/2$ . This result is intuitive.

Mathematicians Only: prolonged scenes of intense rigor.

### 18.1. Chapter Starter Question

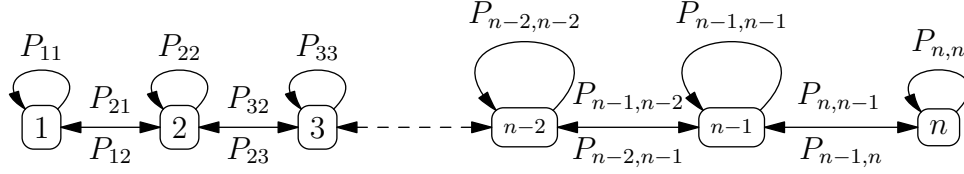
If an irreducible aperiodic Markov chain is symmetric, that is, represented by a symmetric matrix, then what is the specific stationary distribution? What determines the rate at which the Markov chain approaches the stationary distribution?

### 18.2. Introduction, Motivation, Application

Consider a network (or mathematical graph) with  $n \geq 2$  vertices, labeled  $1, 2, \dots, n$  with  $n - 1$  edges connecting adjacent vertices and with a loop at each vertex, as in Figure 18.1. Consider the Markov chain, or random walk, on this graph, with transition probability from vertex  $i$  to vertex  $j$  denoted  $P_{ij}$ . The requirement that transitions can occur only on an edge or loop of the graph is equivalent to  $P_{ij} = 0$  when  $|i - j| > 1$ . Thus  $P$  is a tridiagonal matrix. Since  $P_{ij}$  are transition probabilities,  $P_{ij} \geq 0$  and  $\sum_j P_{ij} = 1$ . Since the row sums are 1,  $P$  is a **stochastic matrix**. In matrix-vector terms,

$$(18.1) \quad P\mathbf{1} = \mathbf{1}$$

where  $\mathbf{1}$  is the  $n \times 1$  vector whose entries are all 1. Therefore, 1 is an eigenvalue of the matrix  $P$ .



**Figure 18.1.** A random walk graph with transition probabilities.

Furthermore, assuming the transition probabilities are symmetric, so that  $P_{ij} = P_{ji}$  means  $P$  is a symmetric, doubly-stochastic, tridiagonal matrix. Since  $P\mathbf{1} = \mathbf{1}$ , then  $(1/n)\mathbf{1}^T P = (1/n)\mathbf{1}^T$ , and the uniform distribution is a stationary distribution for the Markov chain.

The asymptotic rate of convergence of the Markov chain to the stationary distribution depends on the second-largest eigenvalue modulus of  $P$ , called the **mixing rate**. Since  $P$  is symmetric, the eigenvalues of  $P$  are real, and bounded in magnitude by 1. Ordering the eigenvalues by nonincreasing magnitude

$$1 = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq -1$$

the mixing rate is

$$\text{mix}(P) = \max_{i=2,\dots,n} |\lambda_i| = \max(\lambda_2, -\lambda_n)$$

See below for more information and proofs. The smaller  $\text{mix}(P)$  is, the faster the Markov chain converges to its stationary distribution.

The following is an application and motivation for this Markov chain. A processor is located at each vertex of the graph. Each edge represents a direct network connection between the adjacent processors. The processor can be a computer in a network or it can be human worker, such as a line of assemblers in a workshop. The line has a constant total amount of work to be done. Each processor has a job load or queue to finish, say processor  $j$  has load  $q_j(t)$  at time  $t$  where  $q_j(t)$  is a positive real number. The load balancing is done in steps *before* any processing or work begins, so the total amount of work to be done is constant. At each step, the goal is shift loads between adjacent vertices to balance the load. In other words the goal is to have  $q_j(t) \rightarrow (1/n) \sum_j q_j(0)$  as fast as possible as  $t \rightarrow \infty$ . The results here show the balance can be accomplished fastest by shifting one-half of the load on each vertex to the adjacent vertices.

### 18.3. Proofs about Fastest Mixing

**Lemma 18.1.** *If  $P$  is an  $n \times n$  symmetric stochastic matrix, then*

$$\text{mix}(P) = \|P - (1/n)\mathbf{1}\mathbf{1}^T\|_2$$

where  $\|\cdot\|_2$  denotes the spectral norm.

**Remark 18.2.** The **spectral norm**, also called the operator norm, is the natural norm of a matrix induced by the  $L^2$  or Euclidean vector norm. The spectral norm is also the maximum singular value of the matrix, that is the square root of the maximum eigenvalue of  $A^H A$  where  $A^H$  is the conjugate transpose.

**Proof.** (1) Note that  $\mathbf{1}$  is the eigenvector of  $P$  associated with the eigenvalue  $\lambda = 1$  by equation (18.1). Also  $((1/n)\mathbf{1}\mathbf{1}^T)\mathbf{1} = \mathbf{1}$ .

(2) Let  $\mathbf{u}^{(2)}, \dots, \mathbf{u}^{(n)}$  be the other  $n - 1$  eigenvectors of  $P$  corresponding to the eigenvalues  $\lambda_2, \dots, \lambda_n$ . Because  $P$  is symmetric, the eigenvectors are orthogonal. Taking the inner product of  $\mathbf{u}^{(j)}$  with eigenvector  $\mathbf{1}$ , observe that  $\sum_{\nu=1}^n u_{\nu}^{(j)} = 0$  for  $j = 2, \dots, n$ . Therefore

$$((1/n)\mathbf{1}\mathbf{1}^T)\mathbf{u}^{(j)}(1/n)\mathbf{1}(\mathbf{1}^T\mathbf{u}^{(j)}) = 0.$$

(3) Then the eigenvalues of  $P - (1/n)\mathbf{1}\mathbf{1}^T$  are  $\lambda_1 = 0, \lambda_2, \dots, \lambda_n$  with eigenvectors  $\mathbf{1}, \mathbf{u}^{(2)}, \dots, \mathbf{u}^{(n)}$  respectively.

(4) Since  $P - (1/n)\mathbf{1}\mathbf{1}^T$  is symmetric, it is equivalent to a diagonal matrix, and its spectral norm is equal to the maximum magnitude of its eigenvalues, i.e.  $\max\{|\lambda_2|, \dots, |\lambda_n|\}$ , which is  $\text{mix}(P)$ . □

**Lemma 18.3.** *If  $P$  is an  $n \times n$  symmetric stochastic matrix and if  $\mathbf{y}$  and  $\mathbf{z}$  in  $\mathbb{R}^n$  satisfy*

$$(18.2) \quad \mathbf{1}^T \mathbf{y} = 0$$

$$(18.3) \quad \|\mathbf{y}\|_2 = 1$$

$$(18.4) \quad (z_i + z_j)/2 \leq y_i y_j \text{ for } i, j \text{ with } P_{ij} \neq 0$$

then  $\text{mix}(P) \geq \mathbf{1}^T \mathbf{z}$ .

**Proof.** (1) Let the eigenvectors of  $P$  be  $\{\mathbf{u}^{(1)} = \mathbf{1}, \mathbf{u}^{(2)}, \dots, \mathbf{u}^{(n)}\}$ . By the Spectral Theorem these eigenvectors are an orthonormal basis of  $\mathbb{R}^n$ .

(2) Let  $\mathbf{y}$  be as specified in the hypotheses (18.2) and (18.3) and let

$$\mathbf{y} = \sum_{\nu=1}^n \alpha_{\nu} \mathbf{u}^{(\nu)}.$$

(3) By hypothesis (18.3),  $\|\mathbf{y}\|_2 = \sqrt{\sum_{\nu=1}^n \alpha_{\nu}^2} = 1$ .

(4) The eigenvalues of  $P - (1/n)\mathbf{1}\mathbf{1}^T$  are  $\lambda_1 = 0, \lambda_2, \dots, \lambda_n$  with eigenvectors  $\mathbf{1}, \mathbf{u}^{(2)}, \dots, \mathbf{u}^{(n)}$  so

$$(P - (1/n)\mathbf{1}\mathbf{1}^T) \left( \sum_{\nu=1}^n \alpha_{\nu} \mathbf{u}^{(\nu)} \right) = \sum_{\nu=1}^n \alpha_{\nu} \lambda_{\nu} \mathbf{u}^{(\nu)} = \sum_{\nu=2}^n \alpha_{\nu} \lambda_{\nu} \mathbf{u}^{(\nu)}.$$

The last sum on the right side intentionally starts at 2 because the first eigenvalue is 0.

(5) By Lemma 18.1

$$\text{mix}(P) = \|P - (1/n)\mathbf{1}\mathbf{1}^T\|_2.$$

By definition of the spectral norm

$$\|P - (1/n)\mathbf{1}\mathbf{1}^T\|_2 = \max_{\|\mathbf{w}\|=1} \|(P - (1/n)\mathbf{1}\mathbf{1}^T)\mathbf{w}\|_2.$$

- (6) Specializing to the vector  $\mathbf{y}$  with  $\|\mathbf{y}\|_2 = 1$  and using the definition of the 2-norm

$$\begin{aligned}
& \max_{\|\mathbf{w}\|=1} \|(P - (1/n)\mathbf{1}\mathbf{1}^T)\mathbf{w}\|_2 \\
& \geq \|(P - (1/n)\mathbf{1}\mathbf{1}^T)\mathbf{y}\|_2 \\
& = \sqrt{\mathbf{y}^T (P - (1/n)\mathbf{1}\mathbf{1}^T)^T (P - (1/n)\mathbf{1}\mathbf{1}^T) \mathbf{y}} \\
& = \sqrt{\left( \sum_{\nu=1}^n \alpha_{\nu} \mathbf{u}^{(\nu)} \right)^T (P - (1/n)\mathbf{1}\mathbf{1}^T)^T (P - (1/n)\mathbf{1}\mathbf{1}^T) \left( \sum_{\nu=1}^n \alpha_{\nu} \mathbf{u}^{(\nu)} \right)} \\
& = \sqrt{\left( \sum_{\nu=1}^n \alpha_{\nu} \lambda_{\nu} \mathbf{u}^{(\nu)} \right)^T \left( \sum_{\nu=1}^n \alpha_{\nu} \lambda_{\nu} \mathbf{u}^{(\nu)} \right)} \\
& = \sqrt{\sum_{\nu=1}^n \alpha_{\nu}^2 \lambda_{\nu}^2}.
\end{aligned}$$

- (7) Apply Jensen's Inequality to the concave down function  $\sqrt{\cdot}$  over the convex combination defined by  $\alpha_i^2$  which has  $\sum_{i=1}^n \alpha_i^2 = \|\mathbf{y}\|_2 = 1$

$$\sqrt{\sum_{i=1}^n \alpha_i^2 \lambda_i^2} \geq \sum_{i=1}^n \alpha_i^2 |\lambda_i| \geq \sum_{i=1}^n \alpha_i^2 \lambda_i.$$

- (8) Now unwind the expression back into vector notation, again using the orthogonality of the eigenvectors

$$\begin{aligned}
\sum_{\nu=1}^n \alpha_{\nu}^2 \lambda_{\nu} &= \left( \sum_{i=1}^n \alpha_i \mathbf{u}^{(i)} \right)^T (P - (1/n)\mathbf{1}\mathbf{1}^T) \left( \sum_{i=1}^n \alpha_i \mathbf{u}^{(i)} \right) \\
&= \mathbf{y}^T (P - (1/n)\mathbf{1}\mathbf{1}^T) \mathbf{y} \\
&= \mathbf{y}^T P \mathbf{y} \\
&= \sum_{i,j} P_{ij} y_i y_j.
\end{aligned}$$

- (9) Now use the first inequality in step 6 and hypothesis (18.4)

$$\begin{aligned}
\sum_{i,j} P_{ij} y_i y_j &\geq \sum_{i,j} (1/2)(z_i + z_j) P_{ij} \\
&= (1/2)(\mathbf{z}^T P \mathbf{1} + \mathbf{1}^T P \mathbf{z}) \\
&= \mathbf{1}^T \mathbf{z}.
\end{aligned}$$

The second equality follows from the fact that  $P$  is doubly-stochastic. This establishes the lemma.  $\square$

**Lemma 18.4.** *The eigenvalues of the  $n \times n$  tridiagonal matrix*

$$P_{1/2} = \begin{pmatrix} 1/2 & 1/2 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 1/2 & 0 & 1/2 \\ 0 & \cdots & 0 & 1/2 & 1/2 \end{pmatrix}$$

are  $\lambda_1 = 1$  and  $\lambda_j = \cos\left(\frac{(j-1)\pi}{n}\right)$  for  $j = 2, \dots, n$ .

**Remark 18.5.** The following proof is adapted from Feller [Fel73, Section XVI.4]. In fact, Feller finds the eigenvalues and eigenvectors for the more general tridiagonal matrix

$$P_p = \begin{pmatrix} q & p & 0 & \cdots & 0 \\ q & 0 & p & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & q & 0 & p \\ 0 & \cdots & 0 & q & p \end{pmatrix}.$$

The exercises derive the eigenvalues of this more general matrix.

**Proof.** (1) The proof directly finds the eigenvalues permitting solution of the linear system  $P_{1/2}\mathbf{u} = \lambda\mathbf{u}$ . The problem is treated as a linear system in the  $(n-2) \times (n-2)$  system defined by equations  $2, \dots, n-1$  in the variables  $u_2, \dots, u_{n-1}$  and then using the first and last equation as boundary conditions determining values of  $\lambda$  that permit a nontrivial solution.

(2) The equations are

$$(18.5) \quad \lambda u_1 = (1/2)u_1 + (1/2)u_2$$

$$(18.6) \quad \lambda u_j = (1/2)u_{j-1} + (1/2)u_{j+1}, j = 2, \dots, n-1$$

$$(18.7) \quad \lambda u_n = (1/2)u_{n-1} + (1/2)u_n.$$

(3) Equation (18.6) is satisfied by  $u_j = s^j$  provided

$$\lambda s = (1/2) + (1/2)s^2$$

or  $s_+ = \lambda + \sqrt{\lambda^2 - 1}$  and  $s_- = \lambda - \sqrt{\lambda^2 - 1}$ . Then the general solution is of the form  $u_j = A(\lambda)s_+^j + B(\lambda)s_-^j$ .

(4) Apply the first equation ((18.5)) to get

$$\begin{aligned} \lambda(As_+ + Bs_-) &= (1/2)(As_+ + Bs_-) + (1/2)(As_+^2 + Bs_-^2) \\ 0 &= A[(1 - 2\lambda)s_+ + s_+^2] + B[(1 - 2\lambda)s_- + s_-^2] \\ 0 &= A[s_+ - 1] + B[s_- - 1] \\ A[s_+ - 1] &= -B[s_- - 1]. \end{aligned}$$



(5) Apply the last equation (18.7) to get

$$\begin{aligned}
 \text{lambda}(As_+^n + Bs_-^n) &= (1/2)(As_+^{n-1} + Bs_-^{n-1}) + (1/2)(As_+^n + Bs_-^n) \\
 0 &= As_+^{n-1}[1 - 2\text{lambda}s_+ + s_+] + Bs_-^{n-1}[1 - 2\text{lambda}s_- + s_-] \\
 0 &= As_+^{n-1}[-s_+^2 + s_+] + Bs_-^{n-1}[-s_-^2 + s_-] \\
 0 &= As_+^n[-s_+ + 1] + Bs_-^n[-s_- + 1] \\
 -As_+^n[-s_+ + 1] &= Bs_-^n[-s_- + 1] \\
 A[s_+ - 1]s_+^n &= -B[s_- - 1]s_-^n.
 \end{aligned}$$

(6) Combining these equations  $s_+^n = s_-^n$ . Note that  $s_+s_- = 1$ , so  $s_+^{2n} = 1$  and  $s_-^{2n} = 1$ . That is, both  $s_+$  and  $s_-$  are  $2n$ th roots of unity. Therefore,  $s_+$  and  $s_-$  can be written in the form

$$e^{i\pi j/n} = \cos\left(\frac{\pi j}{n}\right) + i \sin\left(\frac{\pi j}{n}\right)$$

for  $j = 0, 1, 2, \dots, 2n - 1$ .

(7) Thus, the eigenvalues  $\text{lambda}$  must be a solution of

$$s_+(\text{lambda}) = e^{i\pi j/n}$$

or

$$\begin{aligned}
 \text{lambda} + \sqrt{\text{lambda}^2 - 1} &= e^{i\pi j/n} \\
 \sqrt{\text{lambda}^2 - 1} &= -\text{lambda} + e^{i\pi j/n} \\
 \text{lambda}^2 - 1 &= \text{lambda}^2 - 2\text{lambda}e^{i\pi j/n} + e^{2i\pi j/n} \\
 -1 &= -2\text{lambda}e^{i\pi j/n} + e^{2i\pi j/n} \\
 \frac{1}{2e^{i\pi j/n}} + \frac{e^{i\pi j/n}}{2} &= \text{lambda} \\
 \frac{e^{-i\pi j/n}}{2} + \frac{e^{i\pi j/n}}{2} &= \text{lambda} \\
 \cos \pi j/n &= \text{lambda}.
 \end{aligned}$$

(8) So to each  $j$  there is a root  $\text{lambda}_j$ , namely

$$\text{lambda}_j = \cos(\pi j/n) \quad j = 0, 1, 2, \dots, 2n - 1.$$

However, some of these roots are repeated, since

$$\cos(\pi j/n) = \cos(\pi(2n - j)/n)$$

for  $j = 1, \dots, n$ . The  $n$  eigenvalues are  $\text{lambda}_1 = 1$  and  $\text{lambda}_j = \cos\left(\frac{(j-1)\pi}{n}\right)$  for  $j = 2, \dots, n$ .

□

**Remark 18.6.** The following lemma is a purely technical lemma about sums of cosines of arithmetic sequences. The next two lemmas use results of this lemma to shorten the proofs.

**Lemma 18.7.** (1) For an integer  $j$

$$\sum_{\ell=1}^n \cos((2\ell-1)(j-1)\pi/n) = 0.$$

(2) In the special case  $j = 2$

$$\sum_{\ell=1}^n \cos((2\ell-1)\pi/n) = 0.$$

(3) For an integer  $j$

$$\sum_{\ell=1}^n \cos^2((2\ell-1)(j-1)\pi/(2n)) = \frac{n}{2}.$$

**Proof.** (1)

$$\begin{aligned} & \sum_{\ell=1}^n \cos((2\ell-1)(j-1)\pi/n) \\ &= \Re \left( \sum_{\ell=1}^n \exp(i(2\ell-1)(j-1)\pi/n) \right) \\ &= \Re \left( \sum_{\ell=1}^n \exp(2\ell(j-1)\pi i/n) \exp(-i(j-1)\pi/n) \right) \\ &= \Re \left( \exp(-i(j-1)\pi/n) \sum_{\ell=1}^n [\exp(2(j-1)\pi i/n)]^\ell \right) \\ &= \Re \left( \exp(-i(j-1)\pi/n) \exp(2(j-1)\pi i/n) \sum_{\ell=1}^n [\exp(2(j-1)\pi i/n)]^{\ell-1} \right) \\ &= \Re \left( \exp(-(j-1)\pi i/n) \exp(2(j-1)\pi i/n) \sum_{\ell=0}^{n-1} [\exp(2(j-1)\pi i/n)]^\ell \right) \\ &= \Re \left( \exp(i(j-1)\pi/n) \frac{1 - [\exp(2(j-1)\pi i/n)]^n}{1 - \exp(2(j-1)\pi i/n)} \right) \\ &= \Re \left( \exp(i(j-1)\pi/n) \frac{1 - \exp(2(j-1)\pi i)}{1 - \exp(2(j-1)\pi i/n)} \right) \\ &= 0. \end{aligned}$$

(2) This is an immediate corollary of the previous with  $j = 2$ .

(3) Use the half-angle formula for the cosine function so

$$\cos^2((2\ell-1)(j-1)\pi/(2n)) = \frac{1}{2} + \cos((2\ell-1)(j-1)\pi/n)$$

and the result follows from the first part.

□

**Lemma 18.8.** *The normalized eigenvectors of the  $n \times n$  tridiagonal matrix*

$$P_{1/2} = \begin{pmatrix} 1/2 & 1/2 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 1/2 & 0 & 1/2 \\ 0 & \cdots & 0 & 1/2 & 1/2 \end{pmatrix}$$

are

$$\begin{aligned} \text{lambd}a_1 &= 1, & \mathbf{u}^{(1)} &= \frac{1}{\sqrt{n}} \mathbf{1} \\ \text{lambd}a_j &= \cos\left(\frac{(j-1)\pi}{n}\right), & u_k^{(j)} &= \sqrt{\frac{2}{n}} \cos\left(\frac{(2k-1)(j-1)\pi}{2n}\right) \end{aligned}$$

for  $j = 2, \dots, n$  and  $k = 1, \dots, n$ .

**Proof.** (1) Since  $P_{1/2}$  is symmetric, already it is established that for  $\text{lambd}a_1 = 1$ , the corresponding normalized eigenvector is  $\mathbf{u}^{(1)} = \frac{1}{\sqrt{n}} \mathbf{1}$ .

(2) For  $j \geq 2$ ,  $\text{lambd}a_j = \cos\left(\frac{(j-1)\pi}{n}\right)$ . The proof of Lemma 18.4 shows the corresponding unnormalized eigenvectors have components

$$u_k^{(j)} = A(\text{lambd}a_j) s_+^k(\text{lambd}a_j) + B(\text{lambd}a_j) s_-^k(\text{lambd}a_j)$$

where  $s_{\pm}(\text{lambd}a_j) = \text{lambd}a_j \pm \sqrt{\text{lambd}a_j^2 - 1} = \cos((j-1)\pi/n) \pm i \sin((j-1)\pi/n) = e^{\pm(j-1)\pi i}$ .

(3) The coefficients  $A(\text{lambd}a_j)$  and  $B(\text{lambd}a_j)$  are determined from the boundary conditions (18.5) and (18.7). But since

$$u_k^{(j)} = A(\text{lambd}a_j) \left[ s_+^k(\text{lambd}a_j) + \frac{B(\text{lambd}a_j)}{A(\text{lambd}a_j)} s_-^k(\text{lambd}a_j) \right]$$

and any scalar multiple of an eigenvector is an eigenvector, only the ratio  $\frac{B(\text{lambd}a_j)}{A(\text{lambd}a_j)}$  is needed.

(4) For notational simplicity, temporarily drop the dependence of  $s_{\pm}$  on  $\text{lambd}a_j$ . Expanding (18.5)

$$2\text{lambd}a A s_+ + 2\text{lambd}a B s_- = A s_+ + B s_- + A s_+^2 + B s_-^2.$$

(5) Rearranging and using  $s_{\pm}^2 - 2\text{lambd}a s_{\pm} = -1$

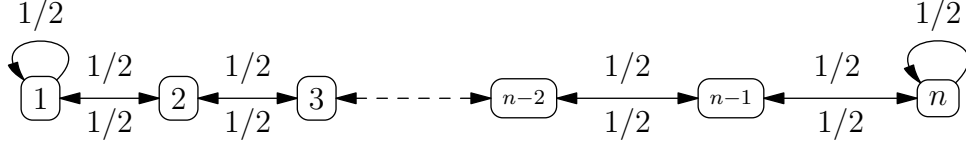
$$\frac{B}{A} = -\frac{s_+ - 1}{s_- - 1}$$

and the components of the unnormalized eigenvector are

$$u_k^{(j)} = \left[ s_+^k(\text{lambd}a_j) - \frac{s_+(\text{lambd}a_j) - 1}{s_-(\text{lambd}a_j) - 1} s_-^k(\text{lambd}a_j) \right].$$

Factoring out  $s_+ - 1$  and remembering that any scalar multiple of an eigenvector is an eigenvector, the components of the unnormalized eigenvector are

$$u_k^{(j)} = \left[ \frac{s_+^k(\text{lambd}a_j)}{s_+(\text{lambd}a_j) - 1} - \frac{s_-^k(\text{lambd}a_j)}{s_-(\text{lambd}a_j) - 1} \right].$$



**Figure 18.2.** The random walk graph with fastest mixing.

- (6) Recalling  $s_{\pm}(\mathbf{lambda}_j) = e^{\pm i(j-1)\pi/n}$ , each fraction can be simplified by multiplying numerator and denominator by the complex conjugate of the denominator

$$\frac{e^{\pm i(j-1)\pi k/n}}{e^{\pm i(j-1)\pi/n} - 1} \cdot \frac{e^{\mp i(j-1)\pi k/n} - 1}{e^{\mp i(j-1)\pi/n} - 1} = \frac{e^{\pm i\pi(j-1)(k-1)/n} - e^{\pm i\pi(j-1)k/n}}{2 - 2\cos(\pi/n)}$$

- (7) Once again remembering that any scalar multiple of an eigenvector is an eigenvector, the constant  $2 - 2\cos(\pi/n)$  in the denominator can be ignored.
- (8) This leaves

$$\begin{aligned} u_k^{(j)} &= (e^{+i(j-1)(k-1)\pi/n} - e^{-i(j-1)(k-1)\pi/n}) - (e^{+i(j-1)k\pi/n} - e^{-i(j-1)k\pi/n}) \\ &= 2\sin((j-1)(k-1)\pi/n) - 2\sin((j-1)k\pi/n) \\ &= 4\sin((j-1)(-1)\pi/(2n))\cos((j-1)(2k-1)\pi/(2n)). \end{aligned}$$

- (9) Finally, factoring out the constant  $-4\sin((j-1)\pi/(2n))$ , the  $k$ th component of the eigenvector corresponding to  $\mathbf{lambda}_j$  is

$$u_k^{(j)} = \cos\left(\frac{(2k-1)(j-1)\pi}{2n}\right).$$

- (10) Using Lemma 18.7, the norm is  $\sqrt{n/2}$  and the  $k$ th component of the normalized eigenvector corresponding to  $\mathbf{lambda}_j$  is

$$u_k^{(j)} = \sqrt{\frac{2}{n}} \cos\left(\frac{(2k-1)(j-1)\pi}{2n}\right).$$

□

**Theorem 18.9.** *The value  $\text{mix}(P_{1/2}) = \cos(\pi/n)$  for*

$$P_{1/2} = \begin{pmatrix} 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1/2 & 0 & 1/2 \\ & & & 1/2 & 1/2 \end{pmatrix}$$

*is the smallest among all symmetric stochastic tridiagonal matrices.*

See Figure 18.2 for the graph associated with this transition probability matrix.

**Proof.** (1) The proof proceeds by constructing a pair of vectors  $\mathbf{y}$  and  $\mathbf{z}$  that satisfy the assumptions of Lemma 18.3 for any symmetric stochastic tridiagonal matrix  $P$ . Furthermore,  $\mathbf{1}^T \mathbf{z} = \cos(\pi/n)$ , so the mixing rate  $\text{mix}(P_{1/2}) = \cos(\pi/n)$  is the fastest possible.

(2) By Lemma 18.4 and the definition of the mixing rate

$$\text{mix}(P_{1/2}) = \lambda_2 = -\lambda_n = \cos(\pi/n).$$

(3) Take  $\mathbf{y} = \mathbf{u}^{(2)}$ , the normalized eigenvector of  $P_{1/2}$  corresponding to  $\lambda_2$ , so the assumptions (18.2) and (18.3) in Lemma 18.3 are automatically satisfied.

(4) Take  $\mathbf{z}$  to be the vector with

$$z_j = \frac{1}{n} \left[ \cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{(2j-1)\pi}{n}\right) \right] / \cos(\pi/n)$$

for  $j = 1, \dots, n$ .

(5) By Lemma 18.7

$$\sum_{j=1}^n \cos((2j-1)\pi/n) = 0.$$

Then  $\mathbf{1}^T \mathbf{z} = \cos(\pi/n)$ .

(6) Now check that  $\mathbf{y}$  and  $\mathbf{z}$  satisfy hypothesis (18.4) of Lemma 18.3.

$$\begin{aligned} \frac{z_j + z_{j+1}}{2} &= \\ &= \frac{1}{n} \left[ \cos\left(\frac{\pi}{n}\right) + \frac{1}{2} \left( \cos\left(\frac{(2j-1)\pi}{n}\right) + \cos\left(\frac{(2j+1)\pi}{n}\right) \right) \right] / \cos(\pi/n). \end{aligned}$$

(7) Using the cosine sum formula

$$\frac{1}{2} \left( \cos\left(\frac{(2j-1)\pi}{n}\right) + \cos\left(\frac{(2j+1)\pi}{n}\right) \right) = \cos\left(\frac{\pi}{n}\right) \cos\left(\frac{2j\pi}{n}\right)$$

this simplifies to

$$\frac{z_j + z_{j+1}}{2} = \frac{1}{n} \left[ \cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{2j\pi}{n}\right) \right].$$

(8) Using the cosine sum formula again

$$\begin{aligned} \frac{z_j + z_{j+1}}{2} &= \frac{1}{n} \left[ \cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{2j\pi}{n}\right) \right] \\ &= \frac{2}{n} \cos\left(\frac{(2j-1)\pi}{2n}\right) \cos\left(\frac{(2j+1)\pi}{2n}\right) \\ &= y_j y_{j+1}. \end{aligned}$$

(9) Therefore *equality* in inequality (18.4) holds for the entries resulting from the nonzero subdiagonal and superdiagonal entries.

(10) For the diagonal entries, check that  $(z_j + z_j)/2 = z_j \leq y_j^2$ . That is, check that

$$\cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{(2j-1)\pi}{n}\right) / \cos\left(\frac{\pi}{n}\right) \leq 2 \cos^2\left(\frac{(2j-1)\pi}{2n}\right).$$

(11) Using the double-angle formula for the cosine

$$2 \cos^2 \left( \frac{(2j-1)\pi}{n} \right) = 1 + \cos \left( \frac{(2j-1)\pi}{n} \right).$$

Therefore, the following inequality needs to be checked

$$\cos \left( \frac{\pi}{n} \right) + \cos \left( \frac{(2j-1)\pi}{n} \right) \Big/ \cos \left( \frac{\pi}{n} \right) \leq 1 + \cos \left( \frac{(2j-1)\pi}{n} \right).$$

(12) Moving all terms to the right the inequality to check is

$$1 - \cos \left( \frac{\pi}{n} \right) - \cos \left( \frac{(2j-1)\pi}{n} \right) \Big/ \cos \left( \frac{\pi}{n} \right) + \cos \left( \frac{(2j-1)\pi}{n} \right) \geq 0.$$

(13) The left side can be factored as

$$\left[ 1 - \cos \left( \frac{\pi}{n} \right) \right] \left[ 1 - \cos \left( \frac{(2j-1)\pi}{n} \right) \Big/ \cos \left( \frac{\pi}{n} \right) \right].$$

(14) This is true because

$$\cos \left( \frac{(2j-1)\pi}{n} \right) \Big/ \cos \left( \frac{\pi}{n} \right) \leq 1$$

for  $j = 1, \dots, n$ .

□

## 18.4. Chapter Ending Answer

Since the transition probability matrix  $P$  is stochastic,  $P\mathbf{1} = \mathbf{1}$ . Since the matrix  $P$  is symmetric,  $\mathbf{1}^T P = \mathbf{1}^T$ . Then normalizing,  $(1/n)\mathbf{1}^T P = (1/n)\mathbf{1}^T$  so the uniform distribution is a stationary distribution. Intuitively, this makes sense since if the matrix is symmetric, the transition probabilities are the same to go from  $i$  to  $j$  as from  $j$  to  $i$ , so the stationary distribution will “even out” to be uniform. The rate of convergence is determined by the eigenvalues, and the eigenvalue with second largest magnitude (since the largest eigenvalue is 1) will dominate the asymptotic rate.

## 18.5. Chapter Summary

### Key Concepts.

- (1) The asymptotic rate of convergence of the Markov chain to the stationary distribution depends on the second-largest eigenvalue modulus, called the mixing rate. The mixing rate is denoted by  $\mu$  or  $\mu(P)$  where  $P$  is the transition probability matrix.
- (2) If  $P$  is an  $n \times n$  symmetric stochastic matrix, then

$$\mu(P) = \|P - (1/n)\mathbf{1}\mathbf{1}^T\|_2$$

where  $\|\cdot\|_2$  denotes the spectral norm.

- (3) The eigenvalues and eigenvectors of the tridiagonal matrix

$$P_{1/2} = \begin{pmatrix} 1/2 & 1/2 & 0 & & \\ 1/2 & 0 & 1/2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1/2 & 0 & 1/2 \\ & & & 1/2 & 1/2 \end{pmatrix}$$

can be determined by solving a recursive system of equations and are  $\lambda_j = \cos\left(\frac{(j-1)\pi}{n}\right)$  for  $j = 1, \dots, n$ . In particular, the largest eigenvalue is 1.

- (4) The mixing rate  $\mu(P_{1/2}) = \cos(\pi/n)$  for  $P_{1/2}$  is the smallest among all symmetric stochastic tridiagonal matrices.

#### Vocabulary.

- (1) A matrix for which the row sums  $\sum_j P_{ij} = 1$  is a **stochastic matrix**.
- (2) The asymptotic rate of convergence of the Markov chain to the stationary distribution depends on the second-largest eigenvalue modulus of  $P$ , called the **mixing rate**.
- (3) The **spectral norm**, also called the operator norm, is the natural norm of a matrix induced by the  $L^2$  or Euclidean vector norm. The spectral norm is also the maximum singular value of the matrix, that is the square root of the maximum eigenvalue of  $A^H A$  where  $A^H$  is the conjugate transpose.

#### Notation.

- (1)  $n$  – number of nodes in the network
- (2)  $i, j$  – typical nodes in the network
- (3)  $P_{ij}$  – transition probability from  $i$  to  $j$
- (4)  $P$  – transition probability matrix
- (5)  $P_{1/2}$  – tridiagonal transition probability matrix with every entry  $1/2$ .
- (6)  $\mathbf{1}$  – the  $n \times 1$  vector whose entries are all 1
- (7)  $1 = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq -1$  – the eigenvalues ordered by nonincreasing magnitude
- (8)  $\text{mix}(P) = \max_{i=2, \dots, n} |\lambda_i(P)| = \max(\lambda_2, -\lambda_n)$  – the mixing rate
- (9)  $A^H$  – conjugate transpose of matrix  $A$
- (10)  $\mathbf{u}^{(2)}, \dots, \mathbf{u}^{(n)}$  – the  $n - 1$  eigenvectors of  $P$  corresponding to the eigenvalues  $\lambda_2, \dots, \lambda_n$
- (11)  $\mathbf{y}, \mathbf{z}$  – vectors in  $\mathbb{R}^n$
- (12)  $s_-, s_+$  – solutions of the quadratic characteristic function.

### 18.6. Sources

This section is adapted from the article by Boyd, Diaconis, Sun and Xiao [BDSX06].

**18.7. Reading Suggestion:****18.8. Outside Readings and Links:**

- (1)
- (2)
- (3)
- (4)

**18.9. Algorithms and Scripts****Data:** Transition probability values**Result:** Eigenvalues of tridiagonal stochastic matrix

**Algorithm.**

```

1 Initialize tridiagonal values for stochastic matrix for  $n = 2 : 8$  do
2   | Build tridiagonal stochastic  $n \times n$  matrix. Calculate eigenvalues of the
   | matrix and display.
3 end

```

**Scripts.****R:** R script for .

```

1   A simple R program using only base functions:
2   \begin{lstlisting}
3   r <- 0
4   p <- 1/2
5   q <- 1 - p
6
7   for (n in 2:8) {
8
9     P <- diag(r, n, n)
10    P[ row(P) - col(P) == 1] <- p
11    P[ row(P) - col(P) == -1] <- q
12    P[1, 1] = q
13    P[n, n] = p
14
15    cat("Size of matrix: ", n , "Eigenvalues: ",
16        unlist(eigen( P, only.values=TRUE )), "\n")
17  }

```

**18.10. Problems to Work for Understanding**

- 1: Show that balancing the workload of a line of processors by shifting one-half of the load on each vertex from the more loaded to the less loaded processor can be represented by the tridiagonal matrix  $P_{1/2}$ .
- 2: Show that  $(1/n) (\mathbf{1}\mathbf{1}^T) \mathbf{1} = \mathbf{1}$ .



3: Devise the exchange rules for an urn model with the  $n \times n$  transition probability matrix  $P_p$ .

4: Show that

$$\frac{1}{2} \left( \cos \left( \frac{(2j-1)\pi}{n} \right) + \cos \left( \frac{(2j+1)\pi}{n} \right) \right) = \cos \left( \frac{\pi}{n} \right) \cos \left( \frac{2j\pi}{n} \right)$$

and

$$\frac{1}{n} \left[ \cos \left( \frac{\pi}{n} \right) + \cos \left( \frac{2j\pi}{n} \right) \right] = \frac{2}{n} \cos \left( \frac{(2j-1)\pi}{2n} \right) \cos \left( \frac{(2j+1)\pi}{2n} \right).$$

5: Show that the four eigenvalues of

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

are  $\cos \left( \frac{(j-1)\pi}{n} \right)$  for  $j = 1, \dots, 4$ .

6: Show that the eigenvalues and for the more general tridiagonal matrix

$$P_p = \begin{pmatrix} q & p & 0 & \cdots & 0 \\ q & 0 & p & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & q & 0 & p \\ 0 & \cdots & 0 & q & p \end{pmatrix}$$

are  $\lambda_1 = 1$  and  $\lambda_j = 2\sqrt{pq} \cos \left( \frac{(j-1)\pi}{n} \right)$  for  $j = 2, \dots, n$ . Then show directly that  $P_{1/2}$  with  $p = q = \frac{1}{2}$  is the fastest mixing among all such tridiagonal matrices  $P$ .

7: Use mathematical software to numerically evaluate the eigenvalues of the matrices  $P_{1/2}$  for sizes  $n = 2, \dots, 8$  and show that the values agree with the exact eigenvalues in Lemma 18.4.

# Introduction to Coupling

*Coupling* means the joint construction of two or more random variables or processes to deduce properties of the individual variables or gain insight into distributional similarities or relations between them.

Mathematicians Only: prolonged scenes of intense rigor.

## 19.1. Chapter Starter Question

What is the Poisson approximation to the binomial distribution with large  $n$  and small  $p$  such that  $np = \lambda$ ? How is the approximation usually proved?

## 19.2. Introduction to Coupling

**Definition 19.1.** A **copy** of a random variable  $X$  is a random variable  $\hat{X}$  with the same distribution as  $X$ ,  $X \stackrel{\mathcal{D}}{=} \hat{X}$ . A **coupling** of a collection of random variables  $X_\nu$ , where  $\nu$  is from some index set  $\mathbb{I}$ , is a similarly indexed set  $(\hat{X}_\nu)$  such that  $X_\nu \stackrel{\mathcal{D}}{=} \hat{X}_\nu$  for each  $\nu$ . The copies  $(\hat{X}_\nu)$  are written in parentheses to indicate the  $\hat{X}_\nu$  random variables have a joint distribution. The definition does *not* require that the joint distribution of  $(\hat{X}_\nu)$  is the same as the joint distribution of the  $X_\nu$ . In fact, it is not even required that a joint distribution of the  $X_\nu$  be specified. A simple and often useful coupling of  $X_\nu$  is  $(\hat{X}_\nu)$  with the  $\hat{X}_\nu$  independent of each other, called the **independence coupling**.  $\diamond$

**Remark 19.2.** Another way to describe the coupling of  $X_\nu$ , where  $\nu$  is from some index set  $\mathbb{I}$ , is a similarly indexed set  $(\hat{X}_\nu)$  with the marginal distribution of each  $\hat{X}_\nu$  the same as the distribution of  $X_\nu$ . Thus, the independence coupling is a valid coupling.

A coupling has fixed marginal distributions given by the  $X_\nu$ . The goal is to find the joint distribution for the coupled variables that satisfies desired properties for proving a theorem or relationship. Many special kinds of couplings exist and

are commonly used for proofs. The independence coupling is the first such special coupling. The propositions below exhibit several other specific kinds of couplings.

Simple preliminary examples of coupling for random variables illustrate the usefulness of coupling. A last example of random variable coupling provides a proof of convergence of a family of Binomial random variables to a Poisson distribution.

**Definition 19.3.** A **self-coupling** of a random variable  $X$  is a family  $(\hat{X}_\nu)$  where each  $\hat{X}_\nu$  is a copy of  $X$ . As a special case of the independence coupling, an **i.i.d. coupling** consists of independent copies of  $X$ .  $\diamond$

**Proposition 19.4.** For every random variable and nondecreasing bounded functions  $f$  and  $g$ , the random variables  $f(X)$  and  $g(X)$  are positively correlated,

$$\text{Cov}[f(X), g(X)] \geq 0.$$

**Proof.** (1) Let  $X'$  be an *independent* copy of  $X$ .

(2) The additivity of covariance shows

$$\begin{aligned} & \text{Cov}[f(X) - f(X'), g(X) - g(X')] = \\ & \text{Cov}[f(X), g(X)] - \text{Cov}[f(X), g(X')] - \text{Cov}[f(X'), g(X)] + \text{Cov}[f(X'), g(X')]. \end{aligned}$$

(3) Since  $X$  and  $X'$  are independent,  $\text{Cov}[f(X), g(X')] = \text{Cov}[f(X'), g(X)] = 0$ . Since  $X$  and  $X'$  have the same distribution,  $\text{Cov}[f(X), g(X)] = \text{Cov}[f(X'), g(X')]$ .

(4) Thus

$$\text{Cov}[f(X), g(X)] = \frac{1}{2} \text{Cov}[f(X) - f(X'), g(X) - g(X')].$$

(5) Since  $\mathbb{E}[f(X) - f(X')] = \mathbb{E}[g(X) - g(X')] = 0$ ,

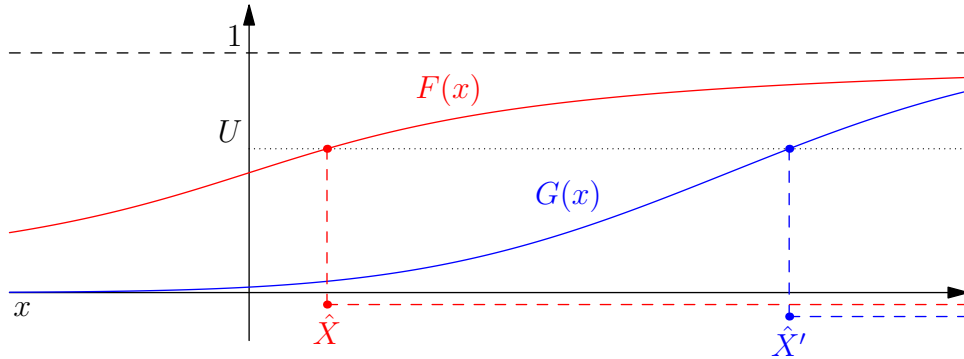
$$\text{Cov}[f(X) - f(X'), g(X) - g(X')] = \mathbb{E}[(f(X) - f(X'))(g(X) - g(X'))].$$

(6) Since  $f$  and  $g$  are nondecreasing,  $f(x) - f(y)$  and  $g(x) - g(y)$  have the same sign for any  $x$  and  $y$ , so  $\mathbb{E}[(f(X) - f(X'))(g(X) - g(X'))] \geq 0$ .  $\square$

**Remark 19.5.** Couplings are useful because a comparison between distributions is reduced to a comparison between random variables. The next few propositions illustrate the idea.

**Definition 19.6.** Let  $X$  be a random variable with c.d.f.  $F$  and  $X'$  be another random variable with c.d.f.  $G$ . If  $G(x) \leq F(x)$  for  $x \in \mathbb{R}$  then  $X$  is said to be **dominated in distribution** by  $X'$ , denoted by  $X \stackrel{\mathcal{D}}{\leq} X'$ . See the schematic diagram in Figure 19.1.  $\diamond$

Let  $X$  be a random variable with c.d.f.  $F$  and  $X'$  be another random variable with c.d.f.  $G$ . If there is a coupling  $(\hat{X}, \hat{X}')$  such that  $\hat{X}$  is *pointwise dominated* by  $\hat{X}'$ , that is,  $\hat{X} \leq \hat{X}'$ , then  $[\hat{X}' \leq x] \subset [\hat{X} \leq x]$ , which implies  $\mathbb{P}[\hat{X}' \leq x] \leq \mathbb{P}[\hat{X} \leq x]$  and thus  $G(x) \leq F(x)$  for  $x \in \mathbb{R}$ .



**Figure 19.1.** Schematic diagram of domination in distribution, pointwise domination and quantile coupling.

**Proposition 19.7.** *Let  $X$  and  $X'$  be random variables. Then  $X \stackrel{\mathcal{D}}{\leq} X'$  if and only if there is a coupling  $(X, X')$  such that  $\hat{X} \leq \hat{X}'$ . In words,  $X$  is dominated in distribution by  $X'$  if and only if there is a coupling such that  $\hat{X}$  is pointwise dominated by  $\hat{X}'$ .*

**Proof.** (1) Let  $U$  be the uniform random variable on  $[0, 1]$ . Then the random variable  $\hat{X} = F^{-1}(U)$  is a copy of  $X$ . Likewise  $\hat{X}' = G^{-1}(U)$  is a copy of  $X'$ . As a side remark, this is called the *quantile coupling*.

(2) Because  $G(x) \leq F(x)$ ,  $u \leq G(x)$  implies  $u \leq F(x)$ .

(3) Thus  $\{x \in \mathbb{R} : u \leq G(x)\} \subset \{x \in \mathbb{R} : u \leq F(x)\}$ .

(4) Thus  $F^{-1}(u) \leq G^{-1}(u)$ , so  $F^{-1}(U) \leq G^{-1}(U)$ . See the schematic diagram in Figure 19.1.

(5) The steps of the proof are reversible, proving the “if and only if”.

□

**Remark 19.8.** The theorem and its proof show that quantile coupling turns domination in distribution into pointwise domination and vice versa. Arguments using pointwise domination are easier than using domination in distribution. The following corollary is an example, since the distribution of a sum, as a convolution of distributions, is harder to use than a sum of random variables.

**Corollary 19.9.** *Let  $X_1, X_2, X'_1, X'_2$  be random variables such that:*

(1)  $X_1$  and  $X_2$  are independent,

(2)  $X'_1$  and  $X'_2$  are independent,

(3)  $X_1 \stackrel{\mathcal{D}}{\leq} X'_1$  and  $X_2 \stackrel{\mathcal{D}}{\leq} X'_2$ .

*Then  $X_1 + X_2 \stackrel{\mathcal{D}}{\leq} X'_1 + X'_2$ .*

**Proof.** (1) Using the Proposition, let  $(\hat{X}_1, \hat{X}'_1)$  be a coupling of  $X_1$  and  $X'_1$  such that  $\hat{X}_1 \stackrel{\mathcal{D}}{\leq} \hat{X}'_1$ .

- (2) Likewise, let  $(\hat{X}_2, \hat{X}'_2)$  be a coupling of  $X_2$  and  $X'_2$  such that  $\hat{X}_2 \stackrel{\mathcal{D}}{\leq} \hat{X}'_2$ .
- (3) Let  $(\hat{X}_1, \hat{X}'_1)$  and  $(\hat{X}_2, \hat{X}'_2)$  be independent.
- (4) Then by definition of having the same distributions,  $(\hat{X}_1 + \hat{X}_2, \hat{X}'_1 + \hat{X}'_2)$  is a coupling of  $X_1 + X_2$  and  $X'_1 + X'_2$ . The independence of  $(\hat{X}_1, \hat{X}'_1)$  and  $(\hat{X}_2, \hat{X}'_2)$  makes it easy to show that  $\hat{X}_1 + \hat{X}_2 \leq \hat{X}'_1 + \hat{X}'_2$ .
- (5) By the Proposition, this implies  $X_1 + X_2 \stackrel{\mathcal{D}}{\leq} X'_1 + X'_2$ .

□

A simple but general and useful tool for coupling is the following theorem.

**Theorem 19.10** (Coupling Inequality). *Let  $X$  and  $Y$  be 2 random variables, each with its own distribution. Then for any subset  $A$*

$$|\mathbb{P}[X \in A] - \mathbb{P}[Y \in A]| \leq \mathbb{P}[X \neq Y].$$

**Proof.** (1) First

$$\begin{aligned} |\mathbb{P}[X \in A] - \mathbb{P}[Y \in A]| &= \\ &= |\mathbb{P}[X \in A, X = Y] + \mathbb{P}[X \in A, X \neq Y] - \\ &\quad - \mathbb{P}[Y \in A, X = Y] - \mathbb{P}[Y \in A, X \neq Y]|. \end{aligned}$$

- (2) But  $\mathbb{P}[X \in A, X = Y] = \mathbb{P}[Y \in A, X = Y]$  since both are the same event, so the two terms cancel.
- (3) Since  $0 \leq \mathbb{P}[X \in A, X \neq Y] \leq \mathbb{P}[X \neq Y]$  and  $0 \leq \mathbb{P}[Y \in A, X \neq Y] \leq \mathbb{P}[X \neq Y]$ , the difference of the two probabilities must be less or equal to  $\mathbb{P}[X \neq Y]$ .
- (4) In summary

$$|\mathbb{P}[X \in A] - \mathbb{P}[Y \in A]| \leq \mathbb{P}[X \neq Y].$$

□

**Proposition 19.11** (Optimal Coupling Equality). *Let  $X$  and  $Y$  be 2 random variables, each with its own distribution. Then for any subset  $A$*

$$\|\text{dist } X - \text{dist } Y\|_{TV} = \inf \{\mathbb{P}[X \neq Y] : (X, Y) \text{ is a coupling of } X, Y\}.$$

*and there is a coupling of  $(X, Y)$  achieving this minimum.*

**Definition 19.12.** The coupling of  $(X, Y)$  achieving this minimum is the **optimal coupling**. ◇

**Proof.** (1) It immediately follows from the definition of the total variation distance and the coupling inequality that

$$\|\text{dist } X - \text{dist } Y\|_{TV} = \inf \mathbb{P}[X \neq Y].$$

- (2) Let

$$p = \sum_{\nu \in \mathcal{X}} \min(\mathbb{P}[X = \nu], \mathbb{P}[Y = \nu]).$$

(3) Write

$$\begin{aligned} \sum_{\nu \in \mathcal{X}} \min(\mathbb{P}[X = \nu], \mathbb{P}[Y = \nu]) \\ = \sum_{\nu \in \mathcal{X}, \mathbb{P}[X = \nu] \leq \mathbb{P}[Y = \nu]} \mathbb{P}[X = \nu] + \sum_{\nu \in \mathcal{X}, \mathbb{P}[X = \nu] > \mathbb{P}[Y = \nu]} \mathbb{P}[Y = \nu]. \end{aligned}$$

(4) Adding and subtracting  $\sum_{\nu \in \mathcal{X}, \mathbb{P}[X = \nu] > \mathbb{P}[Y = \nu]} \mathbb{P}[X = \nu]$  gives

$$\begin{aligned} \sum_{\nu \in \mathcal{X}} \min(\mathbb{P}[X = \nu], \mathbb{P}[Y = \nu]) = \\ 1 - \sum_{\nu \in \mathcal{X}, \mathbb{P}[X = \nu] > \mathbb{P}[Y = \nu]} [\mathbb{P}[X = \nu] - \mathbb{P}[Y = \nu]]. \end{aligned}$$

(5) From one of the equivalent definitions of the total variation metric

$$\sum_{\nu \in \mathcal{X}} \min(\mathbb{P}[X = \nu], \mathbb{P}[Y = \nu]) = 1 - \|\text{dist } X - \text{dist } Y\|_{TV} = p.$$

(6) Flip a coin with probability of heads equal to  $p$ .

(a) If the coin comes up heads, then choose a random value  $Z$  according to the probability distribution

$$\gamma_3(\nu) = \frac{\min \mathbb{P}[X = \nu], \mathbb{P}[Y = \nu]}{p}$$

and set  $X = Y = Z$ .

(b) If the coin comes up tails, choose  $X$  according to the probability distribution

$$\gamma_1(\nu) = \begin{cases} \frac{\mathbb{P}[X = \nu] - \mathbb{P}[Y = \nu]}{\|\text{dist } X - \text{dist } Y\|_{TV}} & \mathbb{P}[X = \nu] > \mathbb{P}[Y = \nu] \\ \text{otherwise} & \end{cases}$$

and independently choose  $Y$  according to the probability distribution

$$\gamma_2(\nu) = \begin{cases} \frac{\mathbb{P}[Y = \nu] - \mathbb{P}[X = \nu]}{\|\text{dist } X - \text{dist } Y\|_{TV}} & \mathbb{P}[Y = \nu] > \mathbb{P}[X = \nu] \\ 0 & \text{otherwise.} \end{cases}$$

(7) By construction  $\gamma_1$  and  $\gamma_2$  are probability distributions and

$$\begin{aligned} p\gamma_3 + (1-p)\gamma_1 &= \text{dist}(X), \\ p\gamma_3 + (1-p)\gamma_2 &= \text{dist}(Y). \end{aligned}$$

(8) In the case that the coin lands tails,  $X \neq Y$  since  $\gamma_1$  and  $\gamma_2$  are positive on disjoint subsets of  $\mathcal{X}$ .

(9) Thus  $X = Y$  if and only if the coin toss is heads. The conclusion is that  $\mathbb{P}[X \neq Y] = \|\text{dist}(X) - \text{dist}(Y)\|_{TV}$ .

□

**Remark 19.13.** Couplings are useful because a comparison between distributions is reduced to a comparison between random variables. For example, the total variation distance  $\|\text{dist}(X) - \text{dist}(Y)\|_{TV}$  is the minimum, over all couplings  $(\hat{X}, \hat{Y})$

of  $X$  and  $Y$ , of the probability that  $X$  and  $Y$  are different. This provides an effective method of obtaining upper bounds on the total variation distance.

A more general version of the optimal coupling theorem is the following.

**Definition 19.14.** Suppose  $(\hat{X}_\nu)$  is a coupling of random variables  $X_\nu$  for  $\nu$  in some index set  $\mathbb{I}$ . If

$$C \subset [\hat{X}_i = \hat{X}_j] \text{ for all } i, j$$

then  $C$  is **coupling event**. ◇

The following lemmas establish the usefulness of the coupling event.

**Lemma 19.15** (Discrete Variable Coupling Event Inequality). *If  $C$  is a coupling event of a family of discrete random variables  $X_\nu$  taking values in a finite or countable set  $E$ , then*

$$\mathbb{P}[C] \leq \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x).$$

**Proof.** (1) Since the random variables are discrete write  $\mathbb{P}[X_\nu = x] = p_\nu(x)$  for the probability mass function.

(2) For all  $i, j \in \mathbb{I}$  and  $x \in E$

$$\mathbb{P}[\hat{X}_i = x, C] = \mathbb{P}[\hat{X}_j = x, C] \leq p_j(x).$$

(3) For all  $i \in \mathbb{I}$  and  $x \in E$

$$\mathbb{P}[\hat{X}_i = x, C] \leq \inf_{j \in \mathbb{I}} p_j(x).$$

(4) Summing over  $E$  gives the inequality. □

**Definition 19.16.** A coupling with a coupling event  $C$  such that

$$\mathbb{P}[C] = \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x)$$

is a **maximal coupling** and  $C$  is a **maximal coupling event**. ◇

**Lemma 19.17.** *Suppose  $X_\nu$  is family of discrete random variables  $X_\nu$  taking values in a finite or countable set  $E$ . Then there exists a maximal coupling.*

**Proof.** (1) From the Coupling Event Inequality, if  $C$  is a coupling event of a family of discrete random variables  $X_\nu$  taking values in a finite or countable set  $E$ , then

$$\mathbb{P}[C] \leq \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x).$$

(2) Let  $c = \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x)$ .

(3) If  $c = 0$ , take the  $\hat{X}_\nu$  independent and the coupling event  $C = \emptyset$ .

(4) If  $c = 1$ , take the  $\hat{X}_\nu$  identical and the coupling event  $C = \Omega$ , the set of all outcomes.

- (5) If  $0 < c < 1$ , mix these two couplings as follows:
- (a)  $U, V, W_\nu, \nu \in \mathbb{I}$  are independent random variables with the following properties.
  - (b)  $U$  is a 0 or 1 valued Bernoulli random variable, with success  $\mathbb{P}[U = 1] = c$ ,
  - (c)  $\mathbb{P}[V = x] = \inf_{\nu \in \mathbb{I}} p_\nu(x)/c$ , for  $x \in E$ ,
  - (d)  $\mathbb{P}[W_\nu = x] = (p_\nu(x) - \mathbb{P}[V = x])/(1 - c)$ , for  $x \in E$ .
- (6) For  $\nu \in \mathbb{I}$

$$\hat{X}_\nu = \begin{cases} V & \text{if } U = 1. \\ W_\nu & \text{if } U = 0. \end{cases}$$

- (7) Then

$$\mathbb{P}[\hat{X}_i = x] = \mathbb{P}[V = x] \mathbb{P}[U = 1] + \mathbb{P}[W_\nu = x] \mathbb{P}[U = 0] = \mathbb{P}[X_\nu = x].$$

- (8) Furthermore,  $C = [U = 1]$  is a coupling event and  $\mathbb{P}[C] = \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x)$ . □

**Example 19.18.** Consider  $n$  Bernoulli trials each with probability  $p$ , or equivalently a binomial distribution  $\text{Bin}(n, p)$  where  $n$  is large and  $p$  is small with  $np = \text{lambda}$ . The Poisson approximation for the probability of  $X$  successes is

$$\mathbb{P}[X = k] = \binom{n}{k} p^k (1-p)^{n-k} \approx e^{-\text{lambda}} \frac{\text{lambda}^k}{k!}$$

is useful. More formally and generally, let  $X_1, \dots, X_n$  be independent Bernoulli, i.e. 0–1, random variables with success  $\mathbb{P}[X_\nu = 1] = p_\nu$  where  $0 \leq p_\nu \leq 1$ . Let  $S_n = X_1 + \dots + X_n$  be the number of successes. If  $\sum_{\nu=1}^n p_\nu \rightarrow \text{lambda}$  while  $\max_{1 \leq \nu \leq n} p_\nu \rightarrow 0$ , then  $S_n \xrightarrow{\mathcal{D}} \text{Pois}(\text{lambda})$ .

The proof by maximal coupling is the following. Let  $X'_1, \dots, X'_n$  be independent Poisson random variables with parameter  $p_\nu$ . Recall that  $X'_1 + \dots + X'_n$  is Poisson with parameter  $p_1 + \dots + p_n = \text{lambda}$ . Let  $(\hat{X}_1, \hat{X}'_1), \dots, (\hat{X}_n, \hat{X}'_n)$  be independent pairs such that for each  $\nu \in 1, \dots, n$ ,  $(\hat{X}_\nu, \hat{X}'_\nu)$  is a maximal coupling of  $X_\nu$  and  $X'_\nu$ . Put

$$\begin{aligned} \hat{X} &= \hat{X}_1 + \dots + \hat{X}_n \\ \hat{X}' &= \hat{X}'_1 + \dots + \hat{X}'_n \end{aligned}$$

so that by Lemma 19.9,  $(\hat{X}, \hat{X}')$  is a coupling of  $X$  and  $X'$  and

$$\mathbb{P}[\hat{X} \neq \hat{X}'] \leq \mathbb{P}[\hat{X}_\nu \neq \hat{X}'_\nu \text{ for some } \nu] \leq \sum_{1 \leq \nu \leq n} \mathbb{P}[\hat{X}_\nu \neq \hat{X}'_\nu].$$

Standard inequalities estimate the sum. Since  $1 + x \leq e^x$  for all  $x$ ,

$$\mathbb{P}[\hat{X}_\nu = 0] = 1 - p_\nu \leq e^{-p_\nu} = \mathbb{P}[\hat{X}'_\nu = 0].$$

Also,

$$\mathbb{P}[\hat{X}_\nu = 1] = p_\nu \geq p_\nu e^{-p_\nu} = \mathbb{P}[\hat{X}'_\nu = 1].$$



Because the coupling is maximal,

$$\begin{aligned}\mathbb{P}[\hat{X}_\nu = \hat{X}'_\nu] &= \min(\mathbb{P}[X_\nu = 0], \mathbb{P}[X'_\nu = 0]) + \min(\mathbb{P}[X_\nu = 1], \mathbb{P}[X'_\nu = 1]) \\ &= 1 - p_\nu + p_\nu e^{-p_\nu}.\end{aligned}$$

Again  $1 - p_\nu \leq e^{-p_\nu}$ , so  $\mathbb{P}[X = X'] \geq 1 - p_\nu^2$  and  $\mathbb{P}[X \neq X'] \leq p_\nu^2$ . Then by the Coupling Inequality the Total Variation distance is less than  $\sum_{\nu=1}^n p_\nu^2$ .

The simplest case is that  $p_\nu \equiv \texttt{lambda}/n$  with  $np_\nu = \texttt{lambda}$ . Then

$$\|\text{Bin}(n, p) - \text{Pois}(\texttt{lambda})\|_{TV} < np^2 = \texttt{lambda}^2/n.$$

Since convergence in Total Variation distance implies convergence in distribution the conclusion follows. A proof of the same result using characteristic functions is in [Bre92, Section 9.4] and [Fel73, Section XI.6] has a proof using generating functions. Both proofs also depend on the inequality  $1 + x \leq e^x$  for all  $x$ .

▽

**Maximal Coupling for Continuous Random Variables.** This section is the continuous analog of the Coupling Inequality and maximal coupling for discrete random variables covered previously. Make the simplifying assumptions that the index set  $\mathbb{I}$  is finite or countable and that each  $X_\nu$  has density  $f_\nu$  so that  $\mathbb{P}[X_\nu \in A] = \int_A f_\nu(x) dx$ .

Suppose  $(\hat{X}_\nu)$  is a coupling of  $X_\nu$  for  $\nu \in \mathbb{I}$  and  $C$  is a coupling event. Then for intervals  $A$  and  $i, j \in \mathbb{I}$ ,

$$\mathbb{P}[\hat{X}_i \in A \cap C] = \mathbb{P}[\hat{X}_j \in A \cap C] \leq \int_A f_j(x) dx.$$

In the case of finite index set  $\mathbb{I}$ , define a partition of  $\mathbb{R}$  by

$$A_1 = \left\{ x \in \mathbb{R} : f_1(x) = \inf_{1 \leq \nu \leq n} f_\nu(x) \right\}$$

and recursively for  $1 < k \leq n$ ,

$$A_k = \left\{ x \in \mathbb{R} : f_k(x) = \inf_{1 \leq \nu \leq n} f_\nu(x) \right\} \setminus (A_1 \cup \dots \cup A_{k-1}).$$

Then

$$\mathbb{P}[\hat{X}_i \in (A \cap A_k) \cap C] \leq \int_{A \cap A_k} f_j(x) dx \leq \int_{A \cap A_k} f_j(x) \inf_{1 \leq \nu \leq n} f_\nu(x) dx$$

where the equality follows from the definition of  $A_k$ . Summing over  $k \in \mathbb{I}$  to obtain the finite case of the Coupling Event Inequality

$$\mathbb{P}[\hat{X}_i \in A \cap C] \leq \int_A \inf_{\nu \in \mathbb{I}} f_\nu.$$

In the countable index set case, fix  $n < \infty$  and use the finite case of the Coupling Event Inequality. Letting  $n \rightarrow \infty$  gives

$$\mathbb{P}[\hat{X}_i \in A \cap C] \leq \int_A \inf_{\nu \in \mathbb{I}} f_\nu$$

because  $\inf_{1 \leq \nu \leq n} f_\nu$  decreases to  $\inf_{\nu \in \mathbb{I}} f_\nu$ . This establishes in either the finite or countable index set case the Coupling Event Inequality.

$$\mathbb{P}[\hat{X}_i \in A \cap C] \leq \int_A \inf_{\nu \in \mathbb{I}} f_\nu.$$

**Theorem 19.19.** Suppose  $X_1, X_2, \dots$  (or  $X_1, X_2, \dots, X_n$ ) are continuous random variable with densities  $f_1, f_2, \dots$  (or  $f_1, f_2, \dots, f_n$ ). Then there exists a maximal coupling with coupling event  $C$  such that  $\mathbb{P}[C] = \int_C \inf_{\nu} f_\nu(x) dx$ .

**Proof.** (1) The proof follows the construction of the maximal coupling for discrete random variables with modifications for the densities instead of discrete probabilities.

(2) Let  $c = \int \inf_{\nu \in \mathbb{I}} f_\nu(x) dx$ .

(3) If  $c = 0$ , take the  $\hat{X}_\nu$  independent and the coupling event  $C = \emptyset$ .

(4) If  $c = 1$ , take the  $\hat{X}_\nu$  identical and the coupling event  $C = \Omega$ , the set of all outcomes.

(5) If  $0 < c < 1$ , mix these two couplings as follows:

- (a)  $U, V, W_\nu, \nu \in \mathbb{I}$  are independent random variables.
- (b)  $U$  is a 0 or 1 valued Bernoulli random variable, with success  $\mathbb{P}[U = 1] = c$ ,
- (c)  $V$  has density  $\inf_{\nu \in \mathbb{I}} f_\nu(x)/c$ ,
- (d)  $W_j$  has density  $f_j(x) - \inf_{\nu \in \mathbb{I}} f_\nu(x)/(1 - c)$ ,

(6) For  $\nu \in \mathbb{I}$

$$\hat{X}_\nu = \begin{cases} V & \text{if } U = 1. \\ W_\nu & \text{if } U = 0. \end{cases}$$

(7) Then

$$\mathbb{P}[\hat{X}_i \in A] = \mathbb{P}[V \in A] \mathbb{P}[U = 1] + \mathbb{P}[W_i \in A] \mathbb{P}[U = 0] = \mathbb{P}[X_i \in A].$$

(8)  $C = [U = 1]$  is a coupling event and  $\mathbb{P}[C] = \int_C \inf_{\nu \in \mathbb{I}} f_\nu(x) dx$  is the value.  $\square$

**Remark 19.20.** Couplings are useful because a comparison between distributions is reduced to a comparison between random variables. For example, the total variation distance  $\|\text{dist}(X) - \text{dist}(Y)\|_{TV}$  is the minimum, over all couplings  $(\hat{X}, \hat{Y})$  of  $X$  and  $Y$  of the probability that  $\hat{X}$  and  $\hat{Y}$  are different. This provides an effective method of obtaining upper bounds on the total variation distance.

**Remark 19.21.** Sometimes it is more convenient to refer to coupling of probability distributions, pushing the corresponding random variables to the background.

### 19.3. Distance from Stationarity

This section is preliminary notation and definitions for later theorems.

Let  $d(t) = \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - \pi\|_{TV}$ . Let  $\bar{d}(t) = \max_{x, y \in \mathcal{X}} \|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV}$ .

**Lemma 19.22.**

$$d(t) \leq \bar{d}(t) \leq 2d(t).$$

**Proof.** (1) From the triangle inequality,  $\bar{d}(t) \leq 2d(t)$ .

(2) To show  $d(t) \leq \bar{d}(t)$ , note first that since  $\pi$  is stationary

$$\sum_{y \in \mathcal{C}} \pi(y) P^t(y, A) = \pi(A)$$

for any set  $A$ .

(3) Then

$$\begin{aligned} |P^t(x, A) - \pi(A)| &= \left| \sum_{y \in \mathcal{C}} \pi(y) [P^t(x, A) - P^t(y, A)] \right| \\ &\leq \sum_{y \in \mathcal{C}} \pi(y) \|P^t(x, A) - P^t(y, A)\|_{TV} \\ &\leq \bar{d}(t) \end{aligned}$$

by the Triangle Inequality and the definition of total variation.

(4) Maximizing over the left side in  $x$  and  $A$  gives  $d(t) \leq \bar{d}(t)$ . □

**Lemma 19.23.** *The function  $\bar{d}$  is submultiplicative,*

$$\bar{d}(s+t) \leq \bar{d}(s)\bar{d}(t).$$

**Proof.** (1) Fix  $x, y \in \mathcal{X}$ .

(2) Let  $(X_s, Y_s)$  be the optimal coupling of  $P^s(x, \cdot)$  and  $P^s(y, \cdot)$ .

(3) Hence  $\|P^s(x, \cdot) - P^s(y, \cdot)\|_{TV} = \mathbb{P}[X_s \neq Y_s]$ .

(4) Then

$$P^{s+t}(x, w) = \sum_{\nu} \mathbb{P}[X_s = z] P^t(z, w) = \mathbb{E}[P^t(X_s, w)].$$

(5) For set  $A$ , summing over  $w \in A$  shows

$$\begin{aligned} P^{s+t}(x, A) - P^{s+t}(y, A) &= \mathbb{E}[P^t(x, A) - P^t(y, A)] \\ &\leq \mathbb{E}[\bar{d}(t)(\mathbf{1}_{X_s \neq Y_s}(\cdot))] = \mathbb{P}[X_s \neq Y_s] \bar{d}(t). \end{aligned}$$

(6) Then using step 3, the right side is at most  $\bar{d}(s)\bar{d}(t)$ . □

**Corollary 19.24.** *If  $\ell$  is a positive integer  $d(\ell t_{\text{mix}}(\epsilon)) \leq \lceil \log_2 \epsilon^{-1} \rceil t_{\text{mix}}$ .*

**Proof.** (1)  $d(\ell t_{\text{mix}}(\epsilon)) \leq \bar{d}(t_{\text{mix}}(\epsilon))^\ell \leq (2\epsilon)^\ell$ .

(2) Taking  $\epsilon = 1/4$ ,  $d(t_{\text{mix}}) \leq 2^{-\ell}$ .

(3) Additionally  $d(\ell t_{\text{mix}}(\epsilon)) \leq \lceil \log_2 \epsilon^{-1} \rceil t_{\text{mix}}$ . □

## 19.4. Coupling for Markov Chains

A simple motivational example introduces coupling of Markov chains.

**Example 19.25.** Consider the Markov chain which is the absorbing symmetric random walk on  $[0, 1, 2, \dots, k]$ . It seems reasonable to conjecture that if  $x < y$ , then  $P^t(x, k) \leq P^t(y, k)$ . That is, the chance of being at the upper absorbing boundary  $k$  after  $t$  steps does not decrease as the starting position increases.

A simple proof uses a coupling of the distributions  $P^t(x, \cdot)$  and  $P^t(y, \cdot)$ . Let  $\Delta_1, \Delta_2, \dots$  be a sequence of i.i.d. Bernoulli random variables taking values  $-1$  with probability  $1/2$  and  $+1$  with probability  $1/2$ . Define two random walks on  $[0, 1, \dots, k]$ , the walk  $(X_t)$  starts at  $x$ , while the walk  $(Y_t)$  starts at  $y$ . Both walks  $(X_t)$  and  $(Y_t)$  move in parallel: if  $\Delta_t = +1$ , move each walk up if possible, and if  $\Delta_t = -1$ , move each walk down if possible. If the two walks meet, necessarily either at  $0$  or  $k$ , they stay together thereafter. The transition probability matrix  $P$  is a  $(k+1) \times (k+1)$  tridiagonal matrix with  $1/2$  on the sub- and super-diagonals,  $1$  at the ends of the main diagonal and  $0$  elsewhere. The distribution of  $X_t$  is  $P^t(x, \cdot)$ , and the distribution of  $Y_t$  is  $P^t(y, \cdot)$ . Importantly,  $X_t$  and  $Y_t$  are defined on the same underlying probability space, as both walks use the sequence  $(\Delta_t)$  to determine their moves. Note that if  $x \leq y$  then  $X_t \leq Y_t$  for all  $t$ . In particular, if  $X_t = k$  then it must be that  $Y_t = k$  also. Conclude that  $P^t(x, k) = \mathbb{P}[X_t = k] \leq \mathbb{P}[Y_t = k] = P^t(y, k)$ . This argument shows how to use coupling to couple together the two walks in such a way that  $X_t \leq Y_t$  pointwise and for all  $t$  and from this fact about the random variables it is easy to gain information about the distributions.  $\nabla$

Building two simultaneous copies of a Markov chain using a common source of randomness, as in the previous example, can be useful for getting bounds on the distance to stationarity.

**Definition 19.26.** Define a **coupling** of Markov chains with transition probability matrix  $P$  to be a process  $(X_t, Y_t)$  for  $t = 0, 1, 2, 3, \dots$  so that both  $(X_t)$  and  $(Y_t)$  are Markov chains with transition probability matrix  $P$ , although the two chains may have different starting distributions.  $\diamond$

**Definition 19.27.** Given a Markov chain on  $\mathcal{X}$  with transition probability matrix  $P$ , a **Markovian coupling** of two  $P$ -chains is a Markov chain  $(X_t, Y_t)$  for  $t = 1, 2, 3, \dots$  with state space  $\mathcal{X} \times \mathcal{X}$  satisfying, for all  $x, y, x', y'$

$$\begin{aligned}\mathbb{P}[X_{t+1} = x' \mid X_t = x, Y_t = y] &= P(x, x') \\ \mathbb{P}[Y_{t+1} = y' \mid Y_t = y, X_t = x] &= P(y, y')\end{aligned}$$

$\diamond$

Not every coupling is a Markovian coupling, as the following example shows.

**Example 19.28.** Let  $\mathcal{X} = \{0, 1\}$  and consider the probability transition probability matrix on  $\mathcal{X}$

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

Let  $(Y_t)$  for  $t = 0, 1, 2, \dots$  be a Markov chain with transition probability matrix  $P$  started in the two states determined by a fair coin toss. Let  $X_0 = 0$  and  $X_{t+1} = Y_t$  for  $t = 0, 1, 2, \dots$ . It is an exercise to show that  $(X_t, Y_t)$  is a coupling, and the sequence  $(X_t, Y_t)$  is a Markov chain but it is not a Markovian coupling.  $\nabla$

If  $(X_t)$  and  $(Y_t)$  are coupled Markov chains with  $X_0 = x$  and  $Y_0 = y$  then use  $\mathbb{P}_{x,y}[\cdot]$  for the probability on the space where  $(X_t)$  and  $(Y_t)$  are both defined.

**Definition 19.29.** Let  $X'$  be a differently started independent version of  $X$  that is,  $X'$  is independent of  $X$  and has the same transition probability matrix but another initial distribution. Let  $\tau_{\text{coal}} \in [1, \infty]$  be the first time the chains meet, that is

$$\tau_{\text{coal}} = \min \{t : X_s = X'_s\}.$$

The time  $\tau_{\text{coal}}$  is called the **coalescence time**, the **coupling time** or the **coupling epoch**.  $\diamond$

**Definition 19.30.** Let  $X''$  the process that follows the path of  $X'$  up to  $\tau_{\text{coal}}$  and then switches to  $X$

$$X''_t = \begin{cases} X'_t & t < \tau_{\text{coal}} \\ X_t & t \geq \tau_{\text{coal}}. \end{cases}$$

By the Markov property, at time  $\tau_{\text{coal}}$  the processes  $X$  and  $X'$  are in the same state and will continue as if they were both starting anew in that state. Thus modifying  $X'$  by switching to  $X$  at time  $\tau_{\text{coal}}$  will not change its distribution, that is,  $X''$  is yet another copy of  $X$ . Thus,  $(X, X'')$  is a coupling of  $X, X'$ , the **classical coupling**. Note carefully the distinct primes and the joint distribution of  $(X, X'')$   $\diamond$

**Theorem 19.31** (Markovian Coupling Inequality). (1) Let  $(X_t, Y_t)$  be a Markovian coupling with  $X_0 = x$  and  $Y_0 = y$

(2) Let  $\tau_{\text{coal}}$  be the coalescence time, that is, the minimum value of  $t$  such that  $X_t = Y_t$

Then

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \mathbb{P}_{x,y}[X_t \neq Y_t] = \mathbb{P}[t < \tau_{\text{coal}}].$$

**Proof.** (1) First observe that  $P^t(x, z) = \mathbb{P}_{x,y}[X_t = z]$  and  $\mathbb{P}_{x,y}[Y_t = z]$  because the coupling is a Markovian coupling.

(2) By the Coupling Inequality

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \mathbb{P}[X_t \neq Y_t].$$

(3) But the event  $[X_t \neq Y_t]$  is precisely the event  $[t < \tau_{\text{coal}}]$  establishing the theorem.  $\square$

**Corollary 19.32.** (1) Let  $(X_t, Y_t)$  be a Markovian coupling with  $X_0 = x$  and  $Y_0 = y$

(2) For each  $x$  and  $y$  Let  $\tau_{x,y,\text{coal}}$  be the coalescence time, that is, the minimum value of  $t$  such that  $X_t = Y_t$ .

Then

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \max_{x,y \in \mathcal{X}} \mathbb{P}_{x,y}[\tau_{x,y,\text{coal}}].$$

**Proof.** Left as an exercise.  $\square$

The coupling is called successful if  $\mathbb{P}[\tau_{coal} < \infty] = 1$ . A successful coupling implies *asymptotic loss of memory*,  $\|xP^t - x'P^t\|_{TV} \rightarrow 0$  at  $t \rightarrow \infty$ . Now the goal is to identify natural conditions on Markov chains that imply successful couplings.

Letting  $\tau_j$  be the first time greater than 0 that the Markov chain visits or returns to  $j$ , recurrence means  $\mathbb{P}_j[\tau_j < \infty] = 1$ . Recall that the Markov chain is called *recurrent* if each state is recurrent. If the Markov chain is irreducible, then  $\mathbb{P}_i[\tau_j < \infty] = 1$  for all initial distributions  $i$  and all states  $j$ . Otherwise, there would be states  $i$  and  $j$  such that  $X$  could go from  $j$  to  $i$  and never return to  $j$ , contradicting the recurrence of  $j$ .

**Example 19.33.** Consider a simple case where the states of both recurrent chains  $X$  and  $X'$  change by  $\pm 1$  on a state space including 0. This would include the alternate Ehrenfest model. Since chains  $X$  and  $X'$  change by  $\pm 1$ ,  $X$  and  $X'$  cannot pass each other without meeting. Thus, if  $X$  starts above  $X'$ , then  $X'$  can hit 0 before the two chains meet. That is,  $\tau_{coal} \leq \tau_0$ . Likewise, if  $X$  starts below  $X'$ , then  $X$  can hit 0 before the two chains meet,  $\tau_{coal} \leq \tau'_0$ . In summary,  $\tau_{coal} \leq \max(\tau_0, \tau'_0)$ . If the chains are recurrent, then the last inequality implies  $\mathbb{P}[\tau_{coal} < \infty] = 1$  and therefore,  $\|xP^t - x'P^t\|_{TV} \rightarrow 0$  at  $t \rightarrow \infty$ .  $\nabla$

The next step shows that recurrence implies the existence of a stationary vector. The proof uses only standard probability arguments, without using coupling. Suppose that  $X$  is a recurrent Markov chain on a finite state space  $\mathcal{X}$  with transition probability matrix  $P$ . Fix an arbitrary state  $j$  and let  $n_i$  be the expected number of steps the chain spends in state  $i$  between visits to state  $j$

$$n_i = \mathbb{E}_j \left[ \sum_{\nu=1}^{\tau_j} \mathbf{1}_{X_\nu=i} \right].$$

The claim is that the row vector  $\mathbf{n}$  with entries  $n_i$  for each  $i \in \mathcal{X}$  is stationary, that is  $\mathbf{n}P^t = \mathbf{n}$ . The claim is established by noting

$$\begin{aligned} n_i &= \mathbb{E}_j \left[ \sum_{\nu=1}^{\tau_j} \mathbf{1}_{X_\nu=i} \right] \\ &= \mathbb{E}_j \left[ \sum_{\nu=1}^{\infty} \mathbf{1}_{X_\nu=i, \tau_j > \nu} \right] \\ &= \sum_{\nu=1}^{\infty} \mathbb{P}[X_\nu = i, \tau_j > \nu]. \end{aligned}$$

It is possible to determine if the event  $[\tau_j > \nu]$  happens or not by observing  $X$  on steps  $1, \dots, \nu$ . By the Markov property, conditionally on the event  $[X_\nu = i, \tau_j > \nu]$ , the process starts over in state  $i$  at time  $\nu$ , that is,

$$P_{i\ell}^t = \mathbb{P}_j[X_{\nu+t} = \ell \mid X_\nu = i, \tau_j > \nu].$$

Then

$$\begin{aligned} n_i P_{i\ell}^t &= \sum_{\nu=1}^{\infty} \mathbb{P}[X_\nu = i, \tau_k > \nu] \cdot \mathbb{P}_k[X_{\nu+t} = j \mid X_\nu = i, \tau_j > \nu] \\ &= \sum_{\nu=1}^{\infty} \mathbb{P}_k[X_{\nu+t} = j, X_\nu = i, \tau_j > \nu]. \end{aligned}$$

Now sum over states  $i$ , recalling that the state space is finite, so interchanging the sums is possible:

$$\begin{aligned} \mathbf{n}P_{\cdot\ell}^t &= \sum_{n=0}^{\infty} \mathbb{P}_k[X_{\nu+t} = \ell, \tau_k > \nu] \\ &= \mathbb{E}_j \left[ \sum_{\nu=0}^{\tau_j} \mathbf{1}_{X_{\nu+t}=\ell} \right] \\ &= \mathbb{E}_j \left[ \sum_{\nu=t}^{\tau_j+t} \mathbf{1}_{X_\nu=\ell} \right] \\ &= \mathbb{E}_j \left[ \sum_{\nu=t}^{\tau_j} \mathbf{1}_{X_\nu=\ell} \right] + \mathbb{E}_j \left[ \sum_{\nu=\tau_k}^{\tau_j+t} \mathbf{1}_{X_\nu=\ell} \right]. \end{aligned}$$

Since  $X$  starts anew in state  $j$  at time  $\tau_j$ , the last summand can be replaced by

$$\mathbb{E}_j \left[ \sum_{\nu=0}^t \mathbf{1}_{X_\nu=\ell} \right].$$

Substituting

$$\begin{aligned} \mathbf{n}P_{\cdot j}^t &= \mathbb{E}_j \left[ \sum_{\nu=t}^{\tau_j} \mathbf{1}_{X_\nu=\ell} \right] + \mathbb{E}_j \left[ \sum_{\nu=0}^t \mathbf{1}_{X_\nu=\ell} \right] \\ &= \mathbb{E}_j \left[ \sum_{\nu=0}^{\tau_j} \mathbf{1}_{X_\nu=\ell} \right] = n_j \end{aligned}$$

Note also that

$$\begin{aligned} \sum_{i \in \mathcal{X}} n_i &= \mathbb{E}_j \left[ \sum_{\nu=0}^{\tau_j} \sum_{i \in \mathcal{X}} \mathbf{1}_{X_\nu=i} \right] \\ &= \mathbb{E}_j \left[ \sum_{\nu=0}^{\tau_k} 1 \right] = \mathbb{E}_j[\tau_j] \end{aligned}$$

The Markov chain is **positive recurrent** if  $m_j = \mathbb{E}_j[\tau_j < \infty]$ . Note that by definition, if a *finite* Markov chain is irreducible, it is necessarily positive recurrent. In this case, the row vector  $\pi = \mathbf{n}/(\sum_\nu n_\nu)$  is a stationary distribution for  $X$ , that is

$$\pi P^t = \pi, \quad \sum_{i \in \mathcal{X}} \pi_i = 1.$$

Now return to using coupling again. Choose the process  $X'$  to be the stationary chain starting from  $\pi$ . Then  $\|xP^t - \pi\|_{TV} \rightarrow 0$  for any starting distribution  $x$ .

### 19.5. Chapter Ending Answer

The Poisson approximation to the binomial distribution with large  $n$  and small  $p$  such that  $np = \text{lambda}$  is

$$\text{Bin}(j; n, p) = \binom{n}{j} p^j (1-p)^{n-j} \approx \frac{\text{lambda}^j}{j!} e^{-\text{lambda}}.$$

A simple proof starts with  $\text{Bin}(0; n, p) = (1-p)^n = \left(1 - \frac{\text{lambda}}{n}\right)^n$ , takes logarithms, uses a Taylor expansion to obtain  $\text{Bin}(j; n, p) \approx \frac{\text{lambda}^j}{j!} e^{-\text{lambda}}$ . Then mathematical induction gives

$$\text{Bin}(j; n, p) = \binom{n}{j} p^j (1-p)^{n-j} \approx \frac{\text{lambda}^j}{j!}.$$

Other typical proofs use characteristic functions and generating functions. This section gives a proof using the idea of coupling to deduce distributional relations between the binomial and Poisson distributions.

### 19.6. Chapter Summary

#### Key Concepts.

- (1) A **coupling** of a collection of random variables  $X_\nu$ , where  $\nu$  is from some index set, is a similarly indexed set  $(\hat{X}_\nu)$  such that  $X_\nu \stackrel{\mathcal{D}}{=} \hat{X}_\nu$  for each  $\nu$ . A coupling has fixed marginal distributions given by the  $X_\nu$ . The goal is to find the joint distribution for the coupled variables that satisfies desired properties for proving a theorem or relationship. Many special kinds of couplings exist and are commonly used for probabilistic proofs.
- (2) Let  $X$  and  $X'$  be random variables. Then  $X \leq X'$  if and only if there is a coupling  $(X, X')$  such that  $\hat{X} \leq \hat{X}'$ . In words,  $X$  is dominated in distribution by  $X'$  if and only if there is a coupling such that  $\hat{X}$  is *pointwise dominated* by  $\hat{X}'$ .
- (3) Let  $X_1, X_2, X'_1, X'_2$  be random variables such that:
  - (a)  $X_1$  and  $X_2$  are independent,
  - (b)  $X'_1$  and  $X'_2$  are independent,
  - (c)  $X_1 \stackrel{\mathcal{D}}{\leq} X'_1$  and  $X_2 \stackrel{\mathcal{D}}{\leq} X'_2$ .
 Then  $X_1 + X_2 \stackrel{\mathcal{D}}{\leq} X'_1 + X'_2$ .
- (4) The Discrete Variable Coupling Event Inequality says that if  $C$  is a coupling event of a family of discrete random variables  $X_\nu$  taking values in a finite or countable set  $E$ , then

$$\mathbb{P}[C] \leq \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x).$$

- (5) A coupling with a coupling event  $C$  such that

$$\mathbb{P}[C] = \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x)$$

is a **maximal coupling** and  $C$  is a **maximal coupling event**.



- (6) Suppose  $X_\nu$  is family of discrete or continuous random variables  $X_\nu$  taking values in a finite or countable set  $E$ . Then there exists a maximal coupling.
- (7) Let  $X_1, \dots, X_n$  be independent Bernoulli, i.e. 0–1, random variables with success  $\mathbb{P}[X_\nu = 1] = p_\nu$  where  $0 \leq p_\nu \leq 1$ . Let  $S_n = X_1 + \dots + X_n$  be the number of successes. If  $\sum_{\nu=1}^n p_\nu \rightarrow \lambda$  while  $\max_{1 \leq \nu \leq n} p_\nu \rightarrow 0$ , then  $S_n \xrightarrow{\mathcal{D}} \text{Pois}(\lambda)$  can be proved using maximal coupling.

### Vocabulary.

- (1) A **copy** of a random variable  $X$  is a random variable  $\hat{X}$  with the same distribution as  $X$ ,  $X \stackrel{\mathcal{D}}{=} \hat{X}$ .
- (2) A **coupling** of a collection of random variables  $X_\nu$ , where  $\nu$  is from some index set  $\mathbb{I}$ , is a similarly indexed set  $(\hat{X}_\nu)$  such that  $X_\nu \stackrel{\mathcal{D}}{=} \hat{X}_\nu$  for each  $\nu$ .
- (3) A simple and often useful coupling of  $X_\nu$  is  $(\hat{X}_\nu)$  with the  $\hat{X}_\nu$  independent, called the **independence coupling**.
- (4) A **self-coupling** of a random variable  $X$  is a family  $(\hat{X}_\nu)$  where each  $\hat{X}_\nu$  is a copy of  $X$ .
- (5) An **i.i.d. coupling** consists of independent copies of  $X$ .
- (6) If  $G(x) \leq F(x)$  for  $x \in \mathbb{R}$  then  $X$  is said to be **dominated in distribution** by  $X'$ , denoted by  $X \stackrel{\mathcal{D}}{\leq} X'$ .
- (7) Suppose  $(\hat{X}_\nu)$  is a coupling of random variables  $X_\nu$  for  $\nu$  in some index set  $\mathbb{I}$ . If

$$C \subset [\hat{X}_i = \hat{X}_j] \text{ for all } i, j$$

then  $C$  is **coupling event**.

- (8) A coupling with a coupling event  $C$  such that

$$\mathbb{P}[C] \leq \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x)$$

is a **maximal coupling** and  $C$  is a **maximal coupling event**.

- (9) The coupling of  $(X, Y)$  achieving the minimum total variation distance is the **optimal coupling**.
- (10) Define a **coupling** of Markov chains with transition probability matrix  $P$  to be a process  $(X_t, Y_t)$  for  $t = 0, 1, 2, 3, \dots$  so that both  $(X_t)$  and  $(Y_t)$  are Markov chains with transition probability matrix  $P$ , although the two chains may have different starting distributions.
- (11) Given a Markov chain on  $\mathcal{X}$  with transition probability matrix  $P$ , a **Markovian coupling** of two  $P$ -chains is a Markov chain  $(X_t, Y_t)$  for  $t = 1, 2, 3, \dots$  with state space  $\mathcal{X} \times \mathcal{X}$  which satisfies, for all  $x, y, x', y'$ ,

$$\mathbb{P}[X_{t+1} = x' \mid X_t = x, Y_t = y] = P(x, x')$$

$$\mathbb{P}[Y_{t+1} = y' \mid Y_t = y, X_t = x] = P(y, y')$$

- (12) The **coalescence time**, the **coupling time** or the **coupling epoch**. – the first time two Markov chains meet, that is

$$\tau_{\text{coal}} = \min \{t : X_s = Y_s\}.$$

- (13) The **classical coupling** – a coupling of  $X$  and  $X''$  that follows the path of  $X'$  up to  $\tau_{\text{coal}}$  and then switches to  $X$ ,

$$X_t'' = \begin{cases} X_t' & t < \tau_{\text{coal}} \\ X_t & t \geq \tau_{\text{coal}}. \end{cases}$$

- (14) The Markov chain is **positive recurrent** if  $m_j = \mathbb{E}_j[\tau_j < \infty]$ .

#### Notation.

- (1)  $\hat{X}$  – a **copy** of a random variable  $X$  with the same distribution as  $X$ ,  $X \stackrel{\mathcal{D}}{=} \hat{X}$ .
- (2)  $\nu$  – an arbitrary index variable
- (3)  $\mathbb{I}$  – index set
- (4)  $(\hat{X}_\nu)$  – copies written in parentheses to indicate the  $\hat{X}_\nu$  random variables have a joint distribution
- (5)  $f$  and  $g$  – nondecreasing bounded functions
- (6)  $F, G$  – c.d.f.s for random variable  $X$  and  $X'$  respectively
- (7)  $X \stackrel{\mathcal{D}}{\leq} X' - G(x) \leq F(x)$  for  $x \in \mathbb{R}$  then  $X$  is said to be **dominated in distribution** by  $X'$
- (8)  $C$  – **coupling event**
- (9)  $c = \sum_{x \in E} \inf_{\nu \in \mathbb{I}} p_\nu(x)$

### 19.7. Sources

The section on coupling random variables is adapted from [Tho00]. The section on coupling in Markov chains is adapted from [LPW09] and [Tho00].

### 19.8. Reading Suggestion:

### 19.9. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)

### 19.10. Algorithms and Scripts

**Input** : Number of balls  $N$  and probability of urn switch,  $p$   
**Output**: Total Variation distance from stationary and empirical probability  $\tau_{\text{coal}} < 10$ .

```

1  $N \leftarrow 7$ ,  $p \leftarrow 1/2$ ,  $q \leftarrow 1 - p$ 
  // Build  $(N + 1) \times (N + 1)$  transition probability matrix
2  $P_{11} \leftarrow q$ ,  $P_{12} \leftarrow p$ 
3  $P_{N+1,N} \leftarrow q$ ,  $P_{N+1,N+1} \leftarrow p$ 
4 for  $r \leftarrow 2$  to  $N$  do
5    $P_{r,r-1} \leftarrow (r - 1)/N \cdot q$ 
6    $P_{r,r} \leftarrow (N - (r - 1))/N \cdot q + (r - 1)/N \cdot p$ 
7    $P_{r,r+1} \leftarrow (N - (r - 1))/N \cdot p$ 
8 end

```

**Algorithm.**

```

  // initialize and build Markov chain
9 Build  $X$  and  $Y$  Markov chain objects
10 Set pathLength, set nTrials, initialize distribution for  $\tau_{\text{coal}}$ 
11 foreach element in nTrials do
12   Run  $X$ ,  $Y$  Markov chains of length pathLength
13   Find  $\tau_{\text{coal}}$ , increment distribution
14 end
15 Normalize distribution
16 Calculate distribution after 10 steps, starting from 0
17 Calculate Total Variation distance from stationary
18 Calculate empirical probability  $\tau_{\text{coal}} < 10$ 
19 Print results for comparison;

```

**Scripts.**

**R:** R script for introcoupling.

```

1 library(markovchain)
2
3 N <- 7
4 p <- 1 / 2
5 q <- 1 - p
6 stateNames <- as.character(0:N)
7 ## Be careful here, because states numbered from 0,
8 ## but R indexes from 1
9 transMatrix <- matrix(0, N + 1, N + 1)
10 transMatrix[1, 1] <- q
11 transMatrix[1, 2] <- p
12 transMatrix[N + 1, N] <- q
13 transMatrix[N + 1, N + 1] <- p
14 for (row in 2:N) {
15   transMatrix[row, row - 1] <- ((row - 1) / N) * q

```

```

16   transMatrix[row, row] <- ((N - (row - 1)) / N) * q
    + ((row - 1) / N) * p
17   transMatrix[row, row + 1] <- ((N - (row - 1)) / N)
    * p
18 }
19
20 stationary <- c(1 / 128, 7 / 128, 21 / 128, 35 / 128,
    35 / 128, 21 / 128, 7 / 128, 1 / 128)
21
22 X <- new("markovchain",
23   states = stateNames,
24   transitionMatrix = transMatrix
25 )
26 Y <- new("markovchain",
27   states = stateNames,
28   transitionMatrix = transMatrix
29 )
30
31 nTrials <- 100
32 pathLength <- 60
33 tauCoalDistribution <- numeric(pathLength + 1)
34 for (i in 1:nTrials) {
35   outsX <- markovchainSequence(pathLength, X, t0 = "0",
    include.t0 = TRUE)
36   outsY <- markovchainSequence(pathLength, Y, include
    .t0 = TRUE) # use stationary
37
38   tauCoal <- min(which(outsX == outsY))
39   if (tauCoal <= pathLength) {
40     tauCoalDistribution[tauCoal] <-
    tauCoalDistribution[tauCoal] + 1
41   }
42 }
43 tauCoalDistribution <- tauCoalDistribution / nTrials
44
45 library(expm)
46 P10_0 <- (transMatrix %^% 10)[1, ]
47 # probability distribution after 10 steps, starting
    from state "0"
48 totVariation <- sum(abs(P10_0 - stationary))
49 # Total Variation distance from stationary of 10
    steps, starting from state "0"
50 coalProb <- sum(tauCoalDistribution[1:10])
51 # \Prob{ \tau_{\text{coal}} < 10 }
52
53 cat("Total Variation Distance after 10 steps,
    starting from state: ", totVariation, "\n")

```

```

54 | cat("Probability Coalescence time less than 10: ",
    | coalProb, "\n")

```

### 19.11. Problems to Work for Understanding

- 1: Let  $\mathcal{X} = \{0, 1\}$  and consider the probability transition probability matrix on  $\mathcal{X}$ :

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

Let  $(Y_t)$  for  $t = 0, 1, 2, \dots$  be a Markov chain with transition probability matrix  $P$  started in one of the two states determined by a fair coin toss. Let  $X_0 = 0$  be in the first state and  $X_{t+1} = Y_t$  for  $t = 0, 1, 2, \dots$ . Show that  $(X_t, Y_t)$  is a coupling, and the sequence  $(X_t, Y_t)$  is a Markov chain but it is not a Markovian coupling.

- 2: Let  $(X_t, Y_t)$  be a Markovian coupling with  $X_0 = x$  and  $Y_0 = y$ . For each  $x$  and  $y$  let  $\tau_{x,y,\text{coal}}$  be the coalescence time, that is, the minimum value of  $t$  such that  $X_t = Y_t$ . Then

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \max_{x,y \in \mathcal{X}} \mathbb{P}_{x,y} [\tau_{x,y,\text{coal}}].$$

## Cutoff Phenomena in Card Shuffling and Random Walks

### 20.1. Rating

An unopened deck of cards has the face-up order (depending on manufacturer, but typically in the U.S.), starting with the Ace of Spades:

- Ace, 2, 3, 4, 5, 6, 7, 8, 9, 10, Jack, Queen, King of Spades,
- Ace, 2, 3, 4, 5, 6, 7, 8, 9, 10, Jack, Queen, King of Diamonds,
- King, Queen, Jack, 10, 9, 8, 7, 6, 5, 4, 3, 2, Ace of Clubs, then
- King, Queen, Jack, 10, 9, 8, 7, 6, 5, 4, 3, 2, Ace of Hearts.

Call this the initial order of the deck. Knowing this order is essential for some sleight of hand tricks performed by a magician. For card players, shuffling the deck to remove this order is essential so that cards dealt from the deck come “at random”, that is, in an order uniformly distributed over all possible deck orders. The main question here is: Starting from this order, how many shuffles are necessary to obtain a “random” deck order from the uniform distribution?

In terms of Markov chains, the questions are: What is the state space, what is an appropriate transition probability matrix, what is the steady state distribution, hopefully uniform, and how fast does the Markov process approach the steady state distribution?

Mathematically Mature: may contain mathematics beyond calculus with proofs.

### 20.2. Chapter Starter Question

Why shuffle a deck of cards? What kind of shuffle do you use? How many shuffles are sufficient to achieve the purpose of shuffling?

### 20.3. General Setting

For simplicity and definiteness, let the cards in the initial deck order

- Ace, 2, 3, 4, 5, 6, 7, 8, 9, 10, Jack, Queen, King of Spades,
- Ace, 2, 3, 4, 5, 6, 7, 8, 9, 10, Jack, Queen, King of Diamonds,
- King, Queen, Jack, 10, 9, 8, 7, 6, 5, 4, 3, 2, Ace of Clubs, then
- King, Queen, Jack, 10, 9, 8, 7, 6, 5, 4, 3, 2, Ace of Hearts.

be numbered 1 to 52. It will also be convenient to study much smaller decks of cards having  $D$  cards. The set of states for a Markov process modeling the order of the deck is  $S_D$ , the set of permutations on  $D$  cards. For convenience, set the initial state  $X_0$  to be the identity permutation with probability 1. In other words, choose the initial distribution as a not yet shuffled deck.

Consider a shuffle, that is, a re-ordering operation on a state that takes an order to another order. For example, the riffle shuffle, also called a dovetail shuffle or leafing the cards, is a common type of shuffle that interleaves packets of cards. A perfect riffle shuffle, also called a faro shuffle, splits the deck exactly in half, then interleaves cards alternately from each half. A perfect riffle shuffle is difficult to perform except for practiced magicians. More commonly, packets of adjacent cards from unevenly split portions interleave, creating a new order for the deck that nevertheless preserves some of the previous order in each packet. Thus a particular riffle shuffle is one of a whole family of riffle shuffles, chosen with a probability distribution on the family. This probability distribution then induces a transition probability from state to state, and thus a Markov process.

Other types of shuffles have colorful names such as the Top-to-Random-Shuffle, Hindu shuffle, pile shuffle, Corgi shuffle, Mongean shuffle, and Weave shuffle. Some shuffle types are a family of possible re-orderings with probability distributions different from the riffle shuffle distribution, leading to different transition probabilities, and thus different Markov processes.

Going from card order  $\pi$  to  $\sigma$  is the same as composing  $\pi$  with the permutation  $\pi^{-1} \circ \sigma$ . Now identify shuffles as functions on  $\{1, \dots, n\}$  to  $\{1, \dots, D\}$ , that is, permutations. Since a particular riffle shuffle is one of a whole family of riffle shuffles, chosen with a probability distribution  $Q$  from the family, the transition probabilities are  $p_{\pi\sigma} = \mathbb{P}[X_{t+1} = \sigma \mid X_t = \pi] = Q(\pi^{-1} \circ \sigma)$ . So now the goal is to describe the probability distribution  $Q$  and apply it to the Markov process.

**Remark 20.1.** This chapter uses a list notation for permutations. For example, the notation  $\pi = [231]$  represents the permutation with  $\pi(1) = 2$ ,  $\pi(2) = 3$  and  $\pi(3) = 1$ . A common alternative matrix notation for the same permutation is

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}.$$

Writing the permutation in matrix form makes finding the inverse obvious,  $\pi^{-1} = [312]$ .

Recall also that sequential permutations are applied from right to left. Composing  $\pi$  with the permutation  $\pi^{-1} \circ \sigma$  gives  $\pi \circ (\pi^{-1} \circ \sigma) = \sigma$ . If  $\sigma = [132]$ , then  $\pi^{-1} \circ \sigma = [321]$  and  $[132] = [231] \circ [321]$ .

This chapter does not use cycle notation for permutations.

## 20.4. Top-to-Random-Shuffle

A particularly simple shuffle is the **Top-to-Random-Shuffle**, abbreviated TTRS. The TTRS takes the top card from a stack of  $D$  cards and inserts it in the gap between the  $(k-1)$ th card and the  $k$ th card in the deck. See Figure 20.1. Note that  $k=1$  is possible, in which case the top card returns to the top. Likewise,  $k=n+1$  is also permitted, in which case the top card moves to the bottom of the card stack.

Consider the order of the cards to be a permutation on  $n$  symbols. The TTRS is naturally a finite Markov chain  $X_t$  for  $t \geq 0$  with  $X_t \in S_n$ . Set  $X_0 = \sigma_0$ , the identity permutation. The transition probabilities are

$$\mathbb{P}[X_{t+1} = \sigma' \mid X_t = \sigma] = \begin{cases} \frac{1}{n} & \sigma' \text{ is a TTRS of } \sigma \\ 0 & \text{otherwise} \end{cases}$$

defining the transition probability matrix  $P$ . Then after  $t$  TTRS shuffles, the order of the deck with  $D$  card has a probability distribution  $X_0 P^t$  on  $S_D$ , where with an overload of notation  $X_0$  is the vector with a 1 in the position for  $\sigma_0$  and 0 elsewhere, representing the initial state. The Markov chain  $X_t$  induced by the TTRS is irreducible, see the exercises. It is also immediate that  $X_t$  is aperiodic since it is possible that the top card can recur back on top. Therefore, this Markov chain must converge to a stationary distribution and this section will later prove that  $X_0 P^t \rightarrow \text{unif}(S_D)$ .

**Example 20.2.** The transition matrix for the TTRS on a deck with three cards is

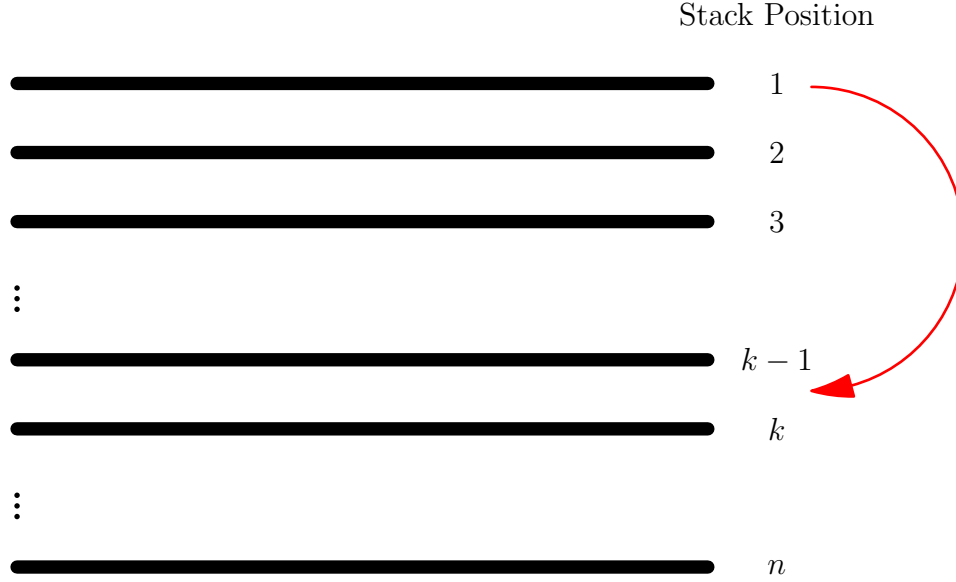
$$\begin{array}{c} [123] \\ [213] \\ [231] \\ [132] \\ [312] \\ [321] \end{array} \begin{pmatrix} [123] & [213] & [231] & [132] & [312] & [321] \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} \end{pmatrix}.$$

If the card deck is initially in order 1 to  $D$  from top to bottom, how many TTRS shuffles does it take for the deck to be sufficiently shuffled? Starting with the identity ordering, the density of the permutations after 7 top-to-random shuffles is the first row of  $P^7$ . Numerically,

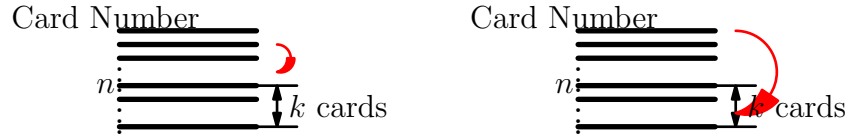
$$P^7 = \begin{pmatrix} 0.16690 & 0.16690 & 0.16690 & 0.16644 & 0.16644 & 0.16644 \\ 0.16690 & 0.16690 & 0.16644 & 0.16690 & 0.16644 & 0.16644 \\ 0.16644 & 0.16644 & 0.16690 & 0.16644 & 0.16690 & 0.16690 \\ 0.16644 & 0.16644 & 0.16644 & 0.16690 & 0.16690 & 0.16690 \\ 0.16690 & 0.16644 & 0.16644 & 0.16690 & 0.16690 & 0.16644 \\ 0.16644 & 0.16690 & 0.16690 & 0.16644 & 0.16644 & 0.16690 \end{pmatrix}.$$

That is, 7 shuffles of the 3-card deck gets close to the stationary density, which turns out to be the uniform density. The eigenvalues of  $P$  are  $1, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, 0$ .





**Figure 20.1.** Schematic drawing of the Top-to-Random-Shuffle.



**Figure 20.2.** Schematic diagram of the proof of the Lemma.

▽

**Lemma 20.3.** *At any time  $t$ , if  $k$  cards appear beneath the card labeled  $D$ , then these cards appear in any order with equal probability.*

**Proof.** The proof is by induction on  $t$ . The base case  $t = 0$  is trivial. Suppose that the claim is true for some  $t > 0$ . In the transition to  $t + 1$ , two cases can occur, see Figure 20.2 for a schematic diagram. First, the top card is randomly placed above the card labeled  $n$  that is somewhere in the stack. Then nothing is changed and the proof is complete. Otherwise, the top card is placed in one of the  $k + 1$  available spaces below the last card (labeled  $n$ ) that is somewhere in the stack. The probability of any particular one of these arrangements is

$$\frac{1}{k!} \cdot \frac{1}{k+1} = \frac{1}{(k+1)!}$$

where  $\frac{1}{k!}$  comes from the induction hypothesis and the  $\frac{1}{k+1}$  comes from the TTRS. The proof is complete.  $\square$

**Theorem 20.4.** Let  $\tau_{\text{top}}$  be the first time that card  $D$  reaches the top of the deck. Then  $X_0 P^{\tau_{\text{top}}+1}$  is uniform on  $S_D$ . Furthermore, whatever permutation arises at time  $\tau_{\text{top}} + 1$  is independent of  $\tau_{\text{top}}$ .

**Proof.** The proof follows from the Lemma, since at time  $\tau_{\text{top}}$  the  $D-1$  cards below card  $D$  will be uniformly distributed over the  $(D-1)!$  possible permutations. Then at time  $\tau_{\text{top}} + 1$  card  $n$  is inserted uniformly at random in the deck.  $\square$

**Remark 20.5.** Waiting for  $\tau_{\text{top}}$  is the same as waiting for completion in the “coupon collectors problem in reverse”. More precisely, collecting a coupon here is putting the top card below the card labeled  $D$ . The first card is hard to put under  $D$ , in fact it happens with probability  $\frac{1}{n+1}$  but it gets easier with more shuffles. This motivates the later assertions that  $\mathbb{E}[\tau_{\text{top}} + 1] = \Theta(n \log n)$  and that  $\mathbb{P}[\tau_{\text{top}} + 1 \geq n \log n + cn] \leq e^{-c}$  for all  $c \geq 0$ . See below for more details.

**Definition 20.6.** If  $\mu$  and  $\nu$  are probability distributions on  $\Omega$ , the **total variation distance** of  $\mu$  from  $\nu$  is

$$\|\mu - \nu\|_{TV} = \sup_{A \subset \Omega} |\mu(A) - \nu(A)| = \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|.$$

$\diamond$

**Remark 20.7.** Probability distributions  $\mu$  and  $\nu$  are far apart in total variation distance if there is a “bad event”  $A$  such that  $\mu$  and  $\nu$  measure  $A$  differently.

**Remark 20.8.** Recall that a *stopping time* is a rule which tells a stochastic process to “stop” depending on the current value of the process.

**Definition 20.9.** Define the stopping time  $\tau$  as a **strong stationary time** for  $X_t$ ,  $t \geq 0$  if  $X_{\tau+1} \sim \text{unif}(S_D)$ , and  $X_{\tau+1}$  is independent of  $\tau$ .  $\diamond$

**Lemma 20.10.** Let  $Q$  be a probability distribution on a finite group  $G$  inducing an irreducible and aperiodic Markov chain with transition probabilities  $Q(\pi^{-1} \circ \sigma)$  from  $\pi$  to  $\sigma$ . Let  $\tau$  be a strong stationary time for  $Q$  and  $U$  the uniform distribution. Then

$$\|Q^\tau - U\|_{TV} \leq \mathbb{P}[\tau > \ell]$$

for all  $\ell \geq 0$

**Remark 20.11.** The hypotheses irreducible and aperiodic may not be strictly necessary, but occur here because both are common in theorems about Markov chains.

**Proof.** For any  $A \subset G$

$$\begin{aligned} Q^\ell(A) &= \mathbb{P}[X_\ell \in A] \\ &= \sum_{j \leq \ell} \mathbb{P}[X_\ell \in A, \tau = j] + \mathbb{P}[X_\ell \in A, \tau > \ell] \\ &= \sum_{j \leq \ell} U(A) \mathbb{P}[\tau = j] + \mathbb{P}[X_\ell \in A \mid \tau > \ell] \mathbb{P}[\tau > \ell] \\ &= U(A) + (\mathbb{P}[X_\ell \in A \mid \tau > \ell] - U(A)) \mathbb{P}[\tau > \ell] / \end{aligned}$$

Because  $|\mathbb{P}[X_\ell \in A \mid \tau > \ell] - U(A)| \leq 1$  in any case

$$\|Q^\tau - U\|_{TV} \leq \mathbb{P}[\tau > \ell].$$

□

**Lemma 20.12.** *Sample uniformly with replacement from an urn with  $n$  balls. Let  $V$  be the number of draws required until each ball has been drawn at least once. Then*

$$\mathbb{P}[V > n \log n + cn] \leq e^{-c}$$

for  $c \geq 0$  and  $n \geq 1$ .

**Remark 20.13.** The lemma statement is another formulation of the coupon collectors problem. The usual formulation has  $n$  different types of coupons or prizes in a cereal box. On each draw, one obtains a coupon or prize equally likely to be any one of the  $n$  types. The goal is to find the expected number of coupons one needs to gather before obtaining a complete set of at least one of each type.

**Proof.** Let  $m = n \log n + cn$ . For each ball  $b$  let  $A_b$  be the event “ball  $b$  not drawn in the first  $m$  draws”. Then

$$\mathbb{P}[V > m] = \mathbb{P}\left[\bigcup_{b=1}^n A_b\right] \leq \sum_{b=1}^n \mathbb{P}[A_b] = n \left(1 - \frac{1}{n}\right)^m \leq ne^{-m/n} = e^{-c}.$$

See the exercises for a proof of the second inequality. □

For simplicity in what follows, set  $d_P(\ell) = \|P^\ell - U\|_{TV}$ . Then  $d_P(\ell)$  measures how close  $\ell$  repeated shuffles get the deck to being shuffled according to the uniform density.

**Theorem 20.14.** *For the TTRS shuffle, and for  $\epsilon < 1$*

- (1)  $d_P(n \log n + n \log \epsilon^{-1}) \leq \epsilon$  for  $n$  sufficiently large, and
- (2)  $d_P(n \log n - n \log(C\epsilon^{-1})) \geq 1 - \epsilon$  for  $n$  sufficiently large.

**Proof.** (1) Theorem 20.4 shows that  $\tau_{\text{top}}$ , the first time that the original bottom card has come to the top and been inserted into the deck is a strong uniform time for the TTRS.

- (2) The goal is to show that  $\tau_{\text{top}}$  has the same distribution as  $V$  in Lemma 20.12. Then the upper bound follows from Lemma 20.12 and Lemma 20.10.

- (3) Write

$$\tau_{\text{top}} = \tau_1 + (\tau_2 - \tau_1) + \cdots + (\tau_{D-1} - \tau_{D-2}) + (\tau_{\text{top}} - \tau_{D-1})$$

where  $\tau_i$  is the time until card  $i$  is placed under the original bottom card.

- (4) When exactly  $i$  cards are under the original bottom card  $b$ , the chance that the current top card is inserted below  $b$  is  $\frac{i+1}{n}$  and hence the random variable  $(\tau_{i+1} - \tau_i)$  has geometric distribution

$$\mathbb{P}[(\tau_{i+1} - \tau_i) = j] = \frac{i+1}{n} \left(1 - \frac{i+1}{n}\right)^{j-1}$$

for  $j \geq 1$ .

- (5) The random variable  $V$  in Lemma 20.12 can be written as

$$V = (V - V_{n-1}) + (V_{n-1} - V_{n-2}) + \cdots + (V_2 - V_1) + V_1$$

where  $V_i$  is the number of draws required until  $i$  distinct balls have been drawn at least once.

- (6) After  $i$  distinct balls have been drawn, the chance that a draw produces a not-previously-drawn ball is  $\frac{n-i}{n}$ . So  $V_i - V_{i-1}$  has distribution

$$\mathbb{P}[V_i - V_{i-1} = j] = \frac{n-i}{n} \left(1 - \frac{n-i}{n}\right)^{j-1}$$

for  $j \geq 1$ .

- (7) Comparing, the corresponding terms  $(\tau_{i+1} - \tau_i)$  and  $V_{n-i} - V_{(n-i)-1}$  have the same distribution. Since the summands in each sum are independent, it follows that the sums  $\tau$  and  $V$  have the same distribution, as required.
- (8) To prove the lower bound, fix  $j$  and let  $A_j$  be the set of configurations of the deck such that the bottom  $j$  original cards stay in their original relative order with the remaining top cards interspersed in any order. There are  $\binom{D}{j} = \frac{D!}{j!(D-j)!}$  positions to put these  $j$  cards in order, then  $(D-j)!$  arrangements for cards in the top portion of the deck, out of  $D!$  total arrangements of, so the uniform distribution probability of  $A_j$  is  $U(A_j) = \frac{1}{j!}$ .
- (9) Let  $\ell(n) = n \log n - c_n n$  where  $c_n \rightarrow \infty$ . The goal is to show  $P^{\ell(n)}(A_j) \rightarrow 1$  as  $n \rightarrow \infty$  for fixed  $j$ . Then  $d_P(\ell(n)) \geq \sup_j \{P^{\ell(n)}(A_j) - U(A_j)\} \rightarrow 1$  as  $n \rightarrow \infty$  for fixed  $j$ , establishing the lower bound.
- (10) To prove  $P^{\ell(n)}(A_j) \rightarrow 1$  as  $n \rightarrow \infty$ , note  $P^{\ell(n)}(A_j) \geq \mathbb{P}[\tau_{\text{top}} - \tau_{j-1} > \ell(n)]$  because  $\tau - \tau_{j-1}$  is distributed as the time for the card initially  $j$ th from the bottom to come to the top and be inserted. If this has not happened by time  $\ell(n)$ , then the original bottom  $j$  cards must still be in their relative order at time  $\ell$ .
- (11) It suffices to show that  $\mathbb{P}[\tau_{\text{top}} - \tau_{j-1} \leq \ell] \rightarrow 0$  as  $n \rightarrow \infty$  for fixed  $j$ . This follows from Chebyshev's inequality. Note that

$$\begin{aligned} \mathbb{E}[(\tau_{i+1} - \tau_i)] &= \frac{n}{i+1}, \\ \text{Var}[(\tau_{i+1} - \tau_i)] &= \left(\frac{n}{i+1}\right)^2 \left(1 - \frac{i+1}{n}\right). \end{aligned}$$

- (12) Using the Euler-Maclaurin formula  $H_\nu = \log \nu + \gamma + \frac{1}{2\nu} + \epsilon_\nu$  for the harmonic numbers

$$\mathbb{E}[(\tau_{\text{top}} - \tau_j)] = \sum_{\nu=j}^{n-1} \frac{n}{\nu+1} = n \log n + O(n)$$

where

$$n \left( \log j - \frac{1}{2j} - \frac{1}{8j^2} \right) \leq O(n) \leq n \left( \log j + \frac{1}{2} - \frac{1}{8n^2} \right).$$

(13) Likewise

$$\begin{aligned}
 \text{Var}[(\tau_{\text{top}} - \tau_j)] &= \sum_{\nu=j}^{n-1} \left( \frac{n}{\nu+1} \right)^2 \left( 1 - \frac{\nu+1}{n} \right) \\
 &= n^2 \sum_{\nu=j}^{n-1} \frac{1}{(\nu+1)^2} - \sum_{\nu=j}^{n-1} \frac{n}{\nu+1} \\
 &= n^2 \sum_{\nu=j}^{n-1} \frac{1}{(\nu+1)^2} - (n \log n + O(n)) = O(n^2).
 \end{aligned}$$

(14) Chebyshev's Inequality says the probability that a random variable differs from the mean by more than a quantity  $a$  is less than the variance divided by  $a^2$ :

$$\mathbb{P}[|Z - \mathbb{E}[Z]| \geq a] \leq \frac{\text{Var}[Z]}{a^2}.$$

Applied to the event  $[\tau_{\text{top}} - \tau_{j-1} \leq k]$ , the mean is increasing as  $O(n \log n)$ , so the distance of  $\mathbb{E}[\tau_{\text{top}} - \tau_{j-1}]$  from  $k$  is increasing as  $O(n \log n)$ . The variance is increasing as  $O(n^2)$ , so the upper estimate of probability of  $\mathbb{P}[\tau_{\text{top}} - \tau_{j-1} \leq k]$  from Chebyshev's Inequality is decreasing as

$$\frac{O(n^2)}{O(n \log n)^2} = O((\log n)^{-2}).$$

Thus  $\mathbb{P}[\tau_{\text{top}} - \tau_{j-1} \leq k] \rightarrow 0$  as  $n \rightarrow \infty$ .

□

**Remark 20.15.** The strong stationary time property of  $\tau_{\text{top}}$  played no role in establishing the lower bound. The proof gets lower bounds by guessing some set  $A$  for which  $P^k(A) - U(A)$  should be large and then using

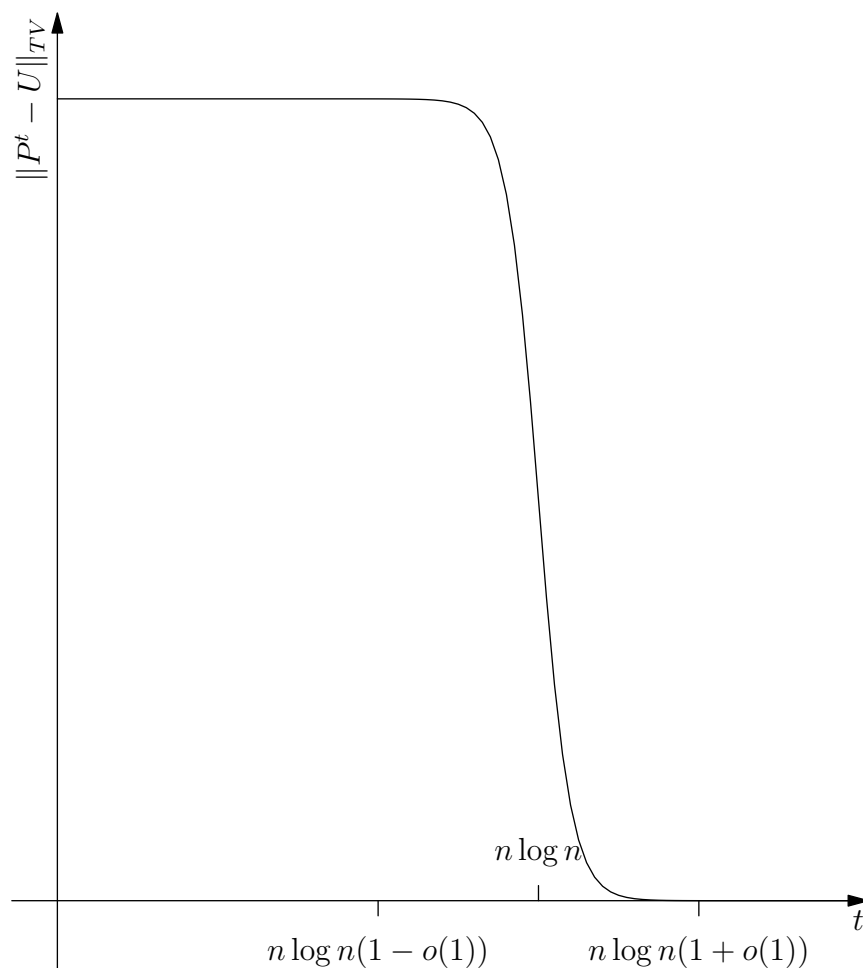
$$d_{\text{top}}(k) = \|P^k - U\|_{\text{TV}} \geq |P^k(A) - U(A)|.$$

Note that  $n \log n + n \log \epsilon^{-1} = n \log n(1 + o(1))$  and  $n \log n - n \log \epsilon^{-1} = n \log n(1 - o(1))$ . This gives the sense that  $n \log n$  shuffles is about the right number of shuffles needed to bring the deck close to being uniformly shuffled. This gives a cut-off phenomenon, that is  $n \log n$  is a critical number of shuffles such that  $d_P(n \log n + o(n)) \approx 0$  but  $d_P(n \log n - o(n)) \approx 1$ . The distance from the stationary density changes abruptly at some value, see Figure 20.3.

**Remark 20.16.** Note that this is quite different from the asymptotics of  $d_P(n) = \|P^n - U\|_{\text{TV}}$ . Perron-Frobenius theory says  $d_P(n) \sim a \lambda^n$  where  $\lambda$  is the second largest eigenvalue, but the long-time asymptotics miss the cut-off.

## 20.5. The Riffle Shuffle

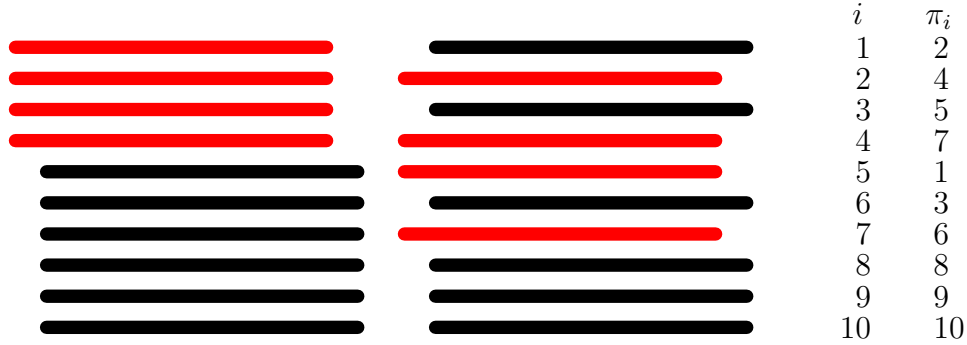
A more realistic model of shuffling a deck cards is the commonly used **riffle shuffle**, occasionally also called the “dovetail shuffle”. This method of randomizing the card order separates the deck into two parts and then leafs through each parts with the thumbs so the cards intermix. The riffle shuffle is sometimes called the GSR shuffle since Gilbert and Shannon and independently Reeds first analyzed it. As a



**Figure 20.3.** Schematic graph of the cut-off phenomenon for the Total Variation distance of the Markov chain distribution from the uniform distribution as a function of the number of steps.

more mathematical description, first cut the deck randomly into two packets, one containing  $\ell$  cards and the other containing  $n - \ell$  cards. Choose the number of cards cut,  $\ell$ , according to the binomial density, meaning that the probability of the cut occurring after  $\ell$  cards is exactly  $\frac{1}{2^n} \binom{n}{\ell}$ .

Once the deck is cut into two packets, interleave the cards from each packet in any possible way, such that the cards from each packet keep their own relative order. This means the cards originally in positions  $1, 2, 3, \dots, \ell$  must still be in the same order after shuffling, even if there are other cards in between. The same goes for cards originally in positions  $\ell + 1, \ell + 2, \dots, n$ . This requirement is quite natural, considering how a person shuffles two packets of cards, one in each hand. The cards from the left hand must still be in the same relative order in the shuffled deck, no matter how they interleave with the cards in the other packet, because the cards



**Figure 20.4.** A riffle shuffle on a 10-card deck cut into a top packet of 4 cards and bottom packet of 6 cards.

drop in order while shuffling. The same goes for the cards in the right hand. See Figure 20.4 for an illustration of a riffle shuffle on a 10-card deck.

Choose among all possible interleavings uniformly with  $\ell$  locations among  $n$  places for the first packet, fixing the locations for the cards of the other packet. This is the well-known “stars and bars” counting argument, with the first packet playing the role of the “stars”, the second packet the “bars” creating  $\binom{n}{\ell}$  possible interleavings. Call this the “uniform interleaving” method. With uniform choice, this means the probability of any one interleaving has probability  $1/\binom{n}{\ell}$  of occurring. Hence the probability of any particular cut, followed by any particular interleaving is  $\frac{1}{2^n} \binom{n}{\ell} \cdot 1/\binom{n}{\ell} = \frac{1}{2^n}$ . Note that this probability has no information about the cut or the interleaving. The density on possible cuts and interleaving is uniform.

A special case of the riffle shuffle is the **perfect shuffle**, also known as the **faro shuffle**, with two equal packets completely interleaved, one card from each hand following one card from the other hand. A perfect shuffle is easy to describe but difficult to perform, except for practiced magicians. The TTRS is also a special case of the riffle shuffle with  $k = 1$  occurring with probability  $n/2^n$ .

A second description of the riffle shuffle is useful for computer scripts simulating the shuffle, see the example in the Scripts section. Begin by choosing a left stack of cards of size  $\ell$  from the top of the deck according to the binomial distribution  $\frac{1}{2^n} \binom{n}{\ell}$ . This creates a right stack of size  $n - \ell$ . Then the cards are dropped from each stack into the shuffled deck with probability proportional to the stack size. Thus, the probability that a card is first dropped from the left stack is  $\ell/n$ . If this happens, the probability that the next card is dropped from the left stack is  $(\ell - 1)/(n - 1)$  and so on. Call this the “left-right drop” method.

**Lemma 20.17.** *The “uniform interleaving” and “left-right drop” methods yield the same probability distribution of shuffles.*

**Proof.** Suppose  $\ell$  cards have been cut off to make the two stacks. For the “uniform interleaving”, a given shuffle is specified by a sequence  $D_1, D_2, \dots, D_n$  where each  $D_i$  is an  $L$  or a  $R$  with  $\ell$  of the  $D_i$ s is  $L$  with probability  $1/\binom{n}{\ell}$ .

**Table 20.1.** Probability distribution for a riffle shuffle on a 3 card deck.

$\pi$	[123]	[213]	[231]	[132]	[312]	[321]
$R(\pi)$	$\frac{1}{2}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	0.

For the “left-right drop”, the sequence  $D_1, D_2, \dots, D_n$  where each  $D_i$  is an  $L$  or a  $R$  with  $\ell$  of the  $D_i$ s is  $L$  occurs with probability (after commuting the probability factors)  $\ell!(n - \ell)!/n!$ .

The two probability distributions are the same.  $\square$

The uniform density on the set of cuts and interleavings now induces in a natural way a density on the set of permutations. Call the density a *riffle shuffle* and denote it by  $R$ . That is,  $R(\pi)$  is the sum of probabilities of each cut and interleaving that gives the rearrangement of the deck corresponding to  $\pi$ . In short, the chance of any arrangement of cards occurring under riffle shuffling is the proportion of cuts and interleavings that give that arrangement.

**Example 20.18.** Consider the riffle shuffle on a 3-card deck as a Markov chain. The probability distribution for  $R$  is in Table 20.1. To obtain the entries in the transition probability matrix, systematically go through the possible cuts and interleavings. Cutting three cards into the left packet, and none in the right packet, the only possible interleaving trivially leaves the deck unchanged. With a cut into 2 cards on the left, 1 card on the right, one interleaving drops the right packet card on the bottom, the left packet cards as the top 2, leaving the deck unchanged. Two other interleavings move the card in the right packet to the middle or the top. The other two cuts are symmetric to the cuts described above, so 4 of the 8 cuts and interleavings keep the deck in the original order. However, one shuffle each moves the formerly bottom card labeled 3 to the middle or top position, leaving cards 1 and 2 in that order in the shuffled deck. A single riffle shuffle cannot reverse the order of the deck.

For the entries in the transition probability matrix, consider the computation for a typical element say  $P_{\pi, \sigma}$  with  $\pi = [213]$  and  $\sigma = [132]$ . Then  $\pi^{-1} = [213]$  and  $\pi^{-1} \circ \sigma = [231]$ . Now  $R([231]) = \frac{1}{8}$ , giving  $P_{[213][132]} = \frac{1}{8}$  in the transition probability matrix.

The full transition probability matrix under this ordering of the permutations is

$$\begin{array}{l}
 [123] \\
 [213] \\
 [231] \\
 [132] \\
 [312] \\
 [321]
 \end{array}
 \begin{pmatrix}
 [123] & [213] & [231] & [132] & [312] & [321] \\
 \frac{1}{2} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & 0 \\
 \frac{1}{8} & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{8} \\
 \frac{1}{8} & \frac{1}{8} & \frac{1}{2} & 0 & \frac{1}{8} & \frac{1}{8} \\
 \frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} \\
 \frac{1}{8} & 0 & \frac{1}{8} & \frac{1}{8} & \frac{1}{2} & \frac{1}{8} \\
 0 & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{2}
 \end{pmatrix}.$$

Although in this case, the  $n = 3$  riffle shuffle, the matrix is symmetric, this is in general not true, the riffle shuffle with deck sizes greater than 3 is nonsymmetric, see the exercises.  $\nabla$



First note that the Markov chain for riffle shuffling is regular, that is, any permutation has a positive probability of appearing after sufficiently many shuffles, see the exercises. In fact, any number of shuffles greater than  $\log_2 n$  will do. Since the riffle shuffle Markov chain is regular, there is a unique stationary density, which is the uniform density on  $S_n$ .

Starting with the identity ordering, the density of the permutations after 7 riffle shuffles is the first row of  $P^7$ . With matrix multiplication, the density is nearly uniform. In fact,

$$P^7 = \begin{pmatrix} 0.17059 & 0.16666 & 0.16666 & 0.16666 & 0.16666 & 0.16278 \\ 0.16666 & 0.17059 & 0.16666 & 0.16666 & 0.16278 & 0.16666 \\ 0.16666 & 0.16666 & 0.17059 & 0.16278 & 0.16666 & 0.16666 \\ 0.16666 & 0.16666 & 0.16278 & 0.17059 & 0.16666 & 0.16666 \\ 0.16666 & 0.16278 & 0.16666 & 0.16666 & 0.17059 & 0.16666 \\ 0.16278 & 0.16666 & 0.16666 & 0.16666 & 0.16666 & 0.17059 \end{pmatrix}.$$

That is, 7 shuffles of the 3-card deck gets close to the stationary density, which turns out to be the uniform density.

## 20.6. Probability of a Permutation Under Riffle Shuffle

Define a **rising sequence** of a permutation as a maximal increasing subsequence within the permutation, potentially with gaps in position. In more detail applied to shuffled decks of cards, say  $x$  is a particular card from the deck. After the position of  $x$ , look for the card labeled  $x + 1$ . If found, repeat the procedure, looking after the  $x + 1$  card for the  $x + 2$  card. Keep going in this manner until it is not possible to find the next card adjacent. Now go back to the original card  $x$  and look for the  $x - 1$  card immediately prior and so on. When done, the subsequence of the permutation containing  $x$  is a rising sequence. A little thought shows that a deck breaks down as a disjoint union of its rising sequences, since the union of any two consecutively increasing subsequences with that element is a rising subsequence.

**Example 20.19.** Suppose that a permutation of a 8 -card deck is 45162378. Start with any card, say 3. Look for 4 and do not find it. Look before the 3 and find 2 and before it, with a gap, find 1. So one of the rising sequences of this permutation is 123. Now start again, this time with 6. After a gap, find 7 and then after it 8. Before 6 with a gap find 5 and then 4. So another rising sequence is 45678. This accounts for all cards and the deck has only two rising sequences. Writing the sequence as 45<sub>1</sub>6<sub>23</sub>78, offsetting the two subsequences, makes this clear.  $\nabla$

**Example 20.20.** The riffle shuffle in Figure 20.4 has two rising sequences,  $\pi(1) < \pi(2) < \pi(3) < \pi(4)$  and  $\pi(5) < \pi(6) < \pi(7) < \pi(8) < \pi(9) < \pi(10)$ .  $\nabla$

**Example 20.21.** Note that 45<sub>1</sub>6<sub>23</sub>78 is a possible result of a riffle shuffle. Here the cut must divide the deck into two packets such that the length of each is the same as the length of the corresponding rising sequence. So if the deck started in the natural order and the deck is cut into 123 on left and 45678 on the right, then the shuffle interleaves by dropping on the bottom 8, then 7, then 3, then 2, then 6, then 1, then 5 and 4, thus obtaining the given top down order through riffing.  $\nabla$

In general, a permutation  $\pi$  of  $n$  cards in original order made by a riffle shuffle will have exactly 2 rising sequences (unless it is the identity with exactly 1 rising sequence). This is a consequence of the definition of a riffle shuffle as a cut and an interleaving. Conversely any permutation of  $n$  cards with 1 or 2 rising sequences can be obtained by a physical shuffle. The lengths of the rising sequences define the size of the cut, the gaps in a subsequence define the interleavings. Therefore a mathematical definition of a riffle shuffle can be made as “a permutation with 1 or 2 rising sequences.” Suppose  $c$  cards are cut off the top. Then there are  $\binom{n}{c}$  possible riffle shuffles, (one of which is the identity shuffle). As in Figure 20.4, after the shuffle, the red and black cards form a binary  $n$ -tuple with  $c$  red cards, there are  $\binom{n}{c}$  such  $n$ -tuples, one of which is the original order. The total number of possible riffle shuffles is

$$1 + \sum_{c=0}^n \left( \binom{n}{c} - 1 \right) = 2^n - n.$$

The next goal is to get similar results about what happens after multiple riffle shuffles. This can be done by considering  $a$ -shuffles. A  **$a$ -shuffle** is another probability density on  $S_n$ . Let  $a$  be any positive integer. Cut the deck into  $a$  packets of nonnegative sizes  $m_1, m_2, \dots, m_a$  with  $m_1 + \dots + m_a = n$  but some of the  $m_i$  may be zero. The probability of this particular packet structure is given by the multinomial density:

$$\frac{1}{a^n} \binom{n}{m_1, m_2, \dots, m_a}.$$

Interleave the cards from each packet in any way, so long as the cards from each packet keep the relative order among themselves. With a fixed packet structure, consider all interleavings equally likely. Count the number of such interleavings as the number of ways of choosing among  $n$  positions in the deck,  $m_1$  places for things of the first type,  $m_2$  places for things of the second type and so on. The count is the multinomial coefficient

$$\binom{n}{m_1, m_2, \dots, m_a}.$$

Hence the probability of a particular rearrangement, i.e. a cut of the deck and an interleaving is

$$\frac{1}{a^n} \binom{n}{m_1, m_2, \dots, m_a} \bigg/ \binom{n}{m_1, m_2, \dots, m_a} = \frac{1}{a^n}.$$

So it turns out that each combination of a particular cut into packets and an interleaving is equally likely, just as in the riffle shuffle. The induced density on the permutations leading to the cuts and shuffles is then called the  $a$ -shuffle, with notation  $R_a$ . The riffle shuffle is just the 2-shuffle, so  $R_2 = R$ .

An equivalent description of the  $a$ -shuffle begins the same way, by cutting the deck into packets multinomially. Then drop cards from the bottom of the packets, one at a time, such that the probability of choosing a particular packet to drop is proportional to the relative size of that packet compared to the number of all cards in the packets. The proof of this description is exactly analogous to the  $a = 2$  case.

A third equivalent description is cutting the deck multinomially into packets of size  $m_1, m_2, \dots, m_n$  and riffing  $m_1$  and  $m_2$  together, meaning choose uniformly

among all interleavings that the keep the relative order of each packet, then riffing the resulting pile with  $m_3$ , then riffing that resulting pile with  $m_4$  and so on.

It turns out that when performing a single  $a$ -shuffle, the probability of achieving a particular permutation  $\pi$  does not depend on the detailed information in  $\pi$ , but only on the number of rising sequences that  $\pi$  has. In other words, the permutations [12534], [34512], [51234], and [23451] have the same probability under any  $a$ -shuffle, since each has exactly two rising sequences.

A useful code based on  $n$ -digit base- $a$  numbers specifies how to make a particular  $a$ -shuffle. Here a “shuffle” indicates a particular way of rearranging the deck, not the probability density on all such rearrangements. Let  $A$  be an  $n$ -digit base- $a$  number. Count the number of 0s in  $A$ , this will be the size of the first packet  $m_1$  in the  $a$ -shuffle. Then  $m_2$  is the number of 1s in  $A$  and so on up to  $m_a$ , the number of  $(a-1)$ s. This cuts the deck into  $a$  packets. Now take the beginning packet of cards of size  $m_1$ . Envision placing these cards on top of all the 0 digits keeping their order as a rising sequence. Do the same for the next packet of size  $m_2$ , placing them on the 1s. Continue up through the  $(a-1)$ s. This particular way of rearranging the cards will then be the particular cut and the interleaving corresponding to  $A$ . Note that the number of such encodings is  $a^n$ .

**Example 20.22.** Let an 8-card deck start in natural order. Let  $A = 23004103$  be the code for a particular 5-shuffle of the 8-card deck. The code has three 0s, one 1, one 2, two 3s and one 4. Thus  $m_1 = 3$ ,  $m_2 = 1$ ,  $m_3 = 1$ ,  $m_4 = 2$  and  $m_5 = 1$ . So cut the deck into 123|4|5|67|8. We put 123 where the 0s are in  $A$ , 4 where the 1 is, 5 where the 2 is, 67 where the 3s are, and 8 where the 4 is. Then get a shuffled deck of 56128437 after applying  $A$  to the natural order.  $\nabla$

This code gives a bijective correspondence between  $n$ -digit base- $a$  numbers and the set of all ways of cutting and interleaving an  $n$ -card deck according to the  $a$ -shuffle. In fact, putting the uniform density on the set of  $n$ -digit base- $a$  numbers transfers to the correct uniform probability density for cutting and interleaving in an  $a$ -shuffle which means the correct density gets induced on  $S_n$ .

**Theorem 20.23.** *The probability of achieving a permutation  $\pi$  when doing an  $a$ -shuffle on an  $n$ -card deck is*

$$\frac{1}{a^n} \binom{n+a-r}{n},$$

where  $r$  is the number of rising sequences in  $\pi$ .

- Proof.** (1) Establish and fix where the  $(a-1)$  cuts occur in an  $a$ -shuffle, then whatever permutations can actually be achieved by interleaving the cards from this cut and packet structure can be achieved in exactly one way: Just drop the cards in exactly the order of the permutation.
- (2) Thus the probability of achieving a particular permutation is the number of possible ways of making cuts that could actually cause that permutation, divided by the total number of ways of making cuts and interleaving for an  $a$ -shuffle.

- (3) Having  $r$  rising sequences in  $\pi$  determines exactly where  $(r - 1)$  of the cuts must have been: between pairs of consecutive cards in the naturally ordered deck such that the first card of the pair ends one rising sequence of  $\pi$ .
- (4) This means that  $(a - 1) - (r - 1) = a - r$  is unspecified, or that free cuts that can go anywhere.
- (5) So count the number of ways of putting  $a - r$  cuts among  $n$  cards. The standard “stars and bars” combinatorial argument counts

$$\binom{n + a - r}{n}$$

ways to do this, i.e. choosing  $n$  places among  $n + (a - r)$ . This is the numerator of the probability.

- (6) The denominator is the number of possible ways to cut and interleave for an  $a$ -shuffle. The encoding of the shuffles as the number of  $n$ -digit base  $a$  numbers gives  $a^n$  ways to do this.

□

**Remark 20.24.** Compare the results of this theorem with the entries of the matrix

$$\begin{array}{c} \begin{matrix} [123] & [213] & [231] & [132] & [312] & [321] \end{matrix} \\ \begin{matrix} [123] \\ [213] \\ [231] \\ [132] \\ [312] \\ [321] \end{matrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & 0 \\ \frac{1}{8} & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{2} & 0 & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & 0 & \frac{1}{8} & \frac{1}{8} & \frac{1}{2} & \frac{1}{8} \\ 0 & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{2} \end{pmatrix} \end{array}.$$

Application of the theorem is easier than counting the shuffles carrying one permutation to another.

## 20.7. Rate of Convergence to Stationary

Recall the modeling of card shuffling as a Markov chain. The initial state  $X_0$  is the identity permutation, that is cards in the initial deck order numbered 1 to  $n$ , with probability 1. A particular riffle shuffle, one of a whole family of riffle shuffles, is chosen with a probability distribution from the family. This probability distribution then induces a transition probability from state to state. Going from card order  $\pi$  to  $\sigma$  is the same as composing  $\pi$  with the permutation  $\pi^{-1} \circ \sigma$ . Now identify shuffles as functions on  $\{1, \dots, n\}$  to  $\{1, \dots, n\}$ , that is, permutations. Since a particular riffle shuffle is one of a whole family of riffle shuffles, chosen with a probability distribution  $Q$  from the family, the transition probabilities are  $p_{\pi\sigma} = \mathbb{P}[X_{t+1} = \sigma \mid X_t = \pi] = Q(\pi^{-1} \circ \sigma)$ .

The rate of convergence of  $X_t$  to the stationary density, measured by the total variation distance or some other metric, is determined by the eigenvalues of the transition matrix. The entries of  $P^k$  are the probabilities of certain permutations

being achieved under  $k$  riffle shuffles. These probabilities are of the form

$$\frac{1}{2^{nk}} \binom{2^k + n - r}{n},$$

for the probability of a permutation with  $r$  rising sequences being achieved after  $k$  riffle shuffles.

Mann [Man94] asserts that the eigenvalues of the transition probability matrix for a single riffle shuffle are exactly  $1, \frac{1}{2}, \frac{1}{4}, \dots, \frac{1}{2^n}$ , see the exercises. The second largest eigenvalue determines the rate of convergence to the stationary distribution. For riffle shuffling, this eigenvalue is  $\frac{1}{2}$ . Once the variation distance gets to the cutoff, it decreases by a factor of approximately  $\frac{1}{2}$  with each shuffle.

**Example 20.25.** The riffle shuffle matrix for the deck of three cards is

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & 0 \\ \frac{1}{8} & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{2} & 0 & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & 0 & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & 0 & \frac{1}{8} & \frac{1}{8} & \frac{1}{2} & \frac{1}{8} \\ 0 & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{2} \end{pmatrix}.$$

The eigenvalues of this matrix are  $1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ . ▽

A comparison of the total variation distance from uniform after  $n$  shuffles for simulations of the TTRS and the riffle shuffle for a 10-card deck is in Figure 20.5. Both show features of the cut-off phenomenon. Naturally, the riffle shuffle converges to uniform faster since it mixes more cards at each step. Note that 7 riffle shuffles suffice to thoroughly mix a 10-card deck.

## 20.8. Random Walk on the Hypercube

This section shows some sharper estimates of the rate of convergence in specific cases by using coupling. Here the case of random walk on the hypercube exhibits tight bounds which can be used to demonstrate the *cut-off* phenomenon.

Let  $\mathbf{Q}^N$  be the  $N$ -dimensional hypercube graph, with vertices or node set

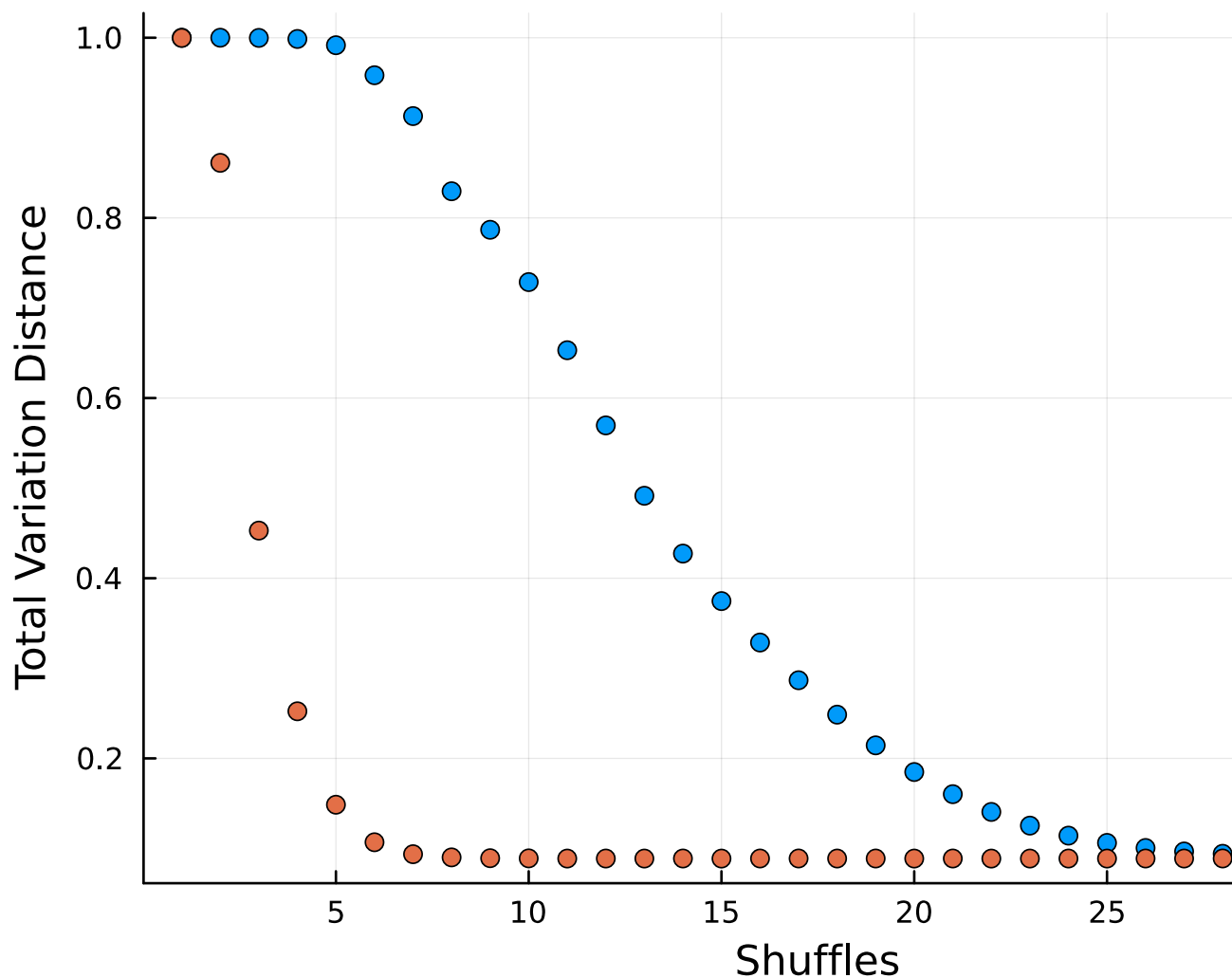
$$V(\mathbf{Q}^N) = \{x_0, x_1, \dots, x_N\} = \{0, 1\}^N$$

and edge set

$$E(\mathbf{Q}^N) = \{(x, y) : x, y \text{ differ in one coordinate}\}.$$

As a notational convenience, let  $\bar{0} = (0, \dots, 0)$  denote the origin and  $\bar{1} = (1, \dots, 1)$  be the extreme vertex of the hypercube.

A random walk on this graph is the sequence  $X_0, X_1, \dots, X_n, X_{n+1}, \dots$  where given  $X_n$ , choose  $X_{n+1}$  uniformly at random from the nodes adjacent to  $X_n$ . A practical way to implement this random walk is to choose a coordinate  $j \in \{1, 2, \dots, N\}$  uniformly at random and flip the bit at  $j$  from 0 to 1 or from 1 to 0. For example, on the 3-dimensional cube a walk at 011 will move to 111 if position 1 is selected, to 001 if position 2 is selected, and 010 if position 3 is selected. As  $n \rightarrow \infty$ , the distribution of  $X_n$  converges to the uniform distribution  $\pi$  on  $V(\mathbf{Q}^N)$ . (See the exercises.) This



**Figure 20.5.** Comparison of the total variation distance from uniform after  $n$  shuffles for the TTRS shuffle in blue and the riffle shuffle in red.

random walk has the annoying disadvantage of being periodic with period 2, so instead consider the *lazy random walk* sequence  $X_0, X_1, \dots, X_n, X_{n+1}, \dots$  where given  $X_n$ , first choose to remain at  $X_n$  with probability  $\frac{1}{2}$ . Alternatively, with probability  $\frac{1}{2}$  choose to move to  $X_{n+1}$  selected uniformly at random from the nodes adjacent to  $x_n$ . A practical way to implement this random walk is to choose a coordinate  $j \in \{1, 2, \dots, N\}$  uniformly at random and replace the bit in that position with the value of a fair Bernoulli random value. The lazy random walk also converges to the uniform distribution  $\pi$  on  $V(\mathbf{Q}^N)$ . (See the exercises.)

The goal is to understand the rate of convergence to the stationary distribution in the Total Variation norm. More precisely, given fixed  $\epsilon$  what the smallest  $t = t(\epsilon)$

such that

$$\|\text{dist}(X_t) - \pi\|_{TV} < \epsilon$$

as a function of  $\epsilon$ ?

The investigation proceeds by coupling. Start one random walk  $X$  at  $\bar{0}$ , and start another random walk  $Y$  “far” from  $\bar{0}$  at  $\bar{1}$ . Define  $\tau = \inf \{t : X_t = Y_t\}$ . Then define a coupled random walk  $X_t = Y_t$  for  $t > \tau$ .

An algorithm to simulate  $X_t$  and  $Y_t$  simultaneously is the following. Given  $X_n = x$  and  $Y_n = y$ , To generate  $X_{n+1}$  and  $Y_{n+1}$ , choose  $j \in \{1, 2, \dots, n\}$  uniformly at random and replace  $x_j$  and  $y_j$  with the *same* random bit chosen as the value of a fair Bernoulli random variable. For example, on the 10-dimensional hypercube suppose the  $X$  random walk is at 0011010011 and the  $Y$  random walk is at 0110001010. Position 6 is selected at random, and the Bernoulli random variable comes up 1. The 6th coordinate is 1, leaving  $X$  unchanged, but the  $Y$  chain moves to 0110011010. This example shows that each of the walks constructed in this way is a lazy random walk on the hypercube.

The following is a general theorem for coupled Markov chains, with a simple proof using the Coupling Inequality. Later, the theorem will be applied to the random walk on the hypercube.

**Theorem 20.26.** (1) Let  $X_t, Y_t$  be coupled Markov chains with  $X_0 = x$  and  $Y_0 = y$ .

(2) Let  $\mathbb{P}_{x,y}[\cdot]$  be the joint probability distribution for  $X_t, Y_t$ .

(3) Let  $\tau_{\text{coal}}$  be the coalescence time of the chains, that is

$$\tau_{\text{coal}} = \min \{t : X_s = Y_s, s \geq t\}.$$

(4) Then

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \mathbb{P}_{x,y}[\tau_{\text{coal}} > t].$$

**Proof.** (1) The first observation is that  $P^t(x, z) = \mathbb{P}_{x,y}[X_t = z]$  and  $P^t(y, z) = \mathbb{P}_{x,y}[Y_t = z]$ .

(2) Using the bound on the total variation metric from the Coupling Inequality

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \mathbb{P}_{x,y}[X_t \neq Y_t].$$

(3) But  $\mathbb{P}_{x,y}[X_t \neq Y_t] = \mathbb{P}_{x,y}[\tau_{\text{coal}} > t]$  which completes the proof. □

Two convenient notations are

$$d(t) = \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - \pi\|_{TV}$$

and

$$\bar{d}(t) = \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV}.$$

**Lemma 20.27.**

$$d(t) \leq \bar{d}(t) \leq 2d(t) \leq 2\bar{d}(t)$$

**Remark 20.28.** These bounds make it clear that to understand the rate of convergence  $d(t)$  (in Total Variation) of the hypercube random walk Markov chain to uniform stationary, understanding  $\bar{d}(t)$  is key. The previous theorem gives a bound on  $\bar{d}(t)$  in terms of  $\mathbb{P}_{x,y}[\tau_{\text{coal}} > t]$ . So following this Lemma, bounding  $\mathbb{P}_{x,y}[\tau_{\text{coal}} > t]$  is the goal.

**Proof.** (1) For the first inequality, start with the simple property of stationarity  $\pi(z) = \sum_{y \in \mathcal{X}} \pi(y) [P^t(y, z)]$ .

(2) Now for any set  $A$  of states, sum the previous over the states  $z \in A$  so  $\pi(A) = \sum_{y \in \mathcal{X}} \pi(y) [P^t(y, A)]$

(3) Using the row sum probability for a Markov chain is 1 and applying absolute values

$$|P^t(x, A) - \pi(A)| = \left| \sum_{y \in \mathcal{X}} \pi(y) [P^t(x, A) - P^t(y, A)] \right|.$$

(4) By the triangle inequality, the definition of total variation distance as the maximum sum of absolute differences over all events, and the definition of  $\bar{d}(t)$ ,

$$\left| \sum_{y \in \mathcal{X}} \pi(y) [P^t(x, A) - P^t(y, A)] \right| \leq \sum_{y \in \mathcal{X}} \pi(y) \|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \bar{d}(t).$$

(5) Maximizing the left side over  $x \in \mathcal{X}$  and  $A$  yields  $d(t) \leq \bar{d}(t)$ .

(6) For the second inequality, start with the triangle inequality for the total variation distance

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \|P^t(x, \cdot) - \pi\|_{TV} + \|\pi - P^t(y, \cdot)\|_{TV}.$$

(7) Then

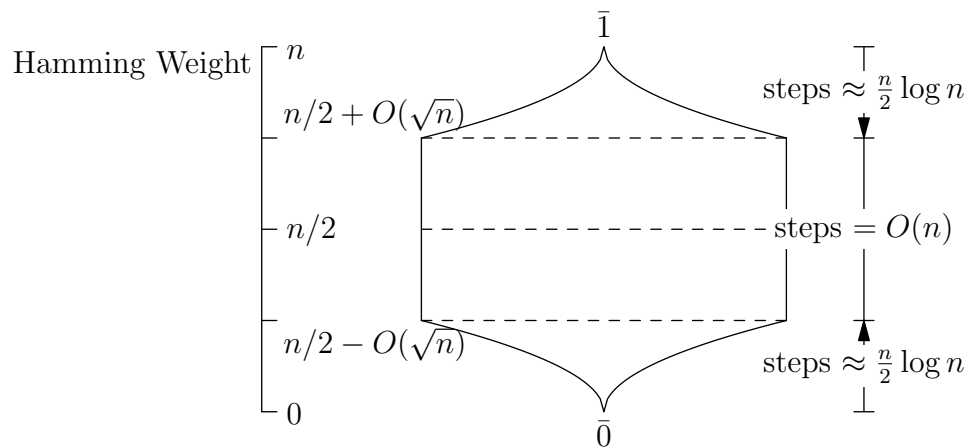
$$\begin{aligned} \bar{d}(t) &= \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \\ &\leq \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - \pi\|_{TV} + \max_{y \in \mathcal{X}} \|\pi - P^t(y, \cdot)\|_{TV} \\ &= 2d(t). \end{aligned}$$

(8) Since the first inequality  $d(t) \leq \bar{d}(t)$  holds, then  $2d(t) \leq 2\bar{d}(t)$  follows immediately. □

Let the **Hamming weight** of a vertex be the sum of the coordinates of the vertex, ranging from Hamming weight 0 at  $\bar{0}$  to  $n$  at  $\bar{1}$ . As notation, use  $\text{ht}(x)$  for the Hamming weight of vertex  $x$ . Consider the schematic characterization of the hypercube in Figure 20.6. The plan for the remainder of the proof is show that both walks  $X_n$  and  $Y_n$  get to the bulk of the hypercube in  $\frac{n}{2} \log n$  steps, and then it takes an additional  $O(n)$  steps for them to meet.

If  $\tau$  is the first time when all the coordinates have been selected at least once, then the two walks agree with each other from time  $\tau$  onward. Let  $R_t$  be the number of unselected coordinates at time  $t$ . Then  $\tau$  is the time that the number of





**Figure 20.6.** Caricature of the hypercube in terms of the Hamming weight of the vertices.

unselected coordinates becomes 0,  $\tau = \min \{t : R_t = 0\}$ . The random variable  $R_t$  decreases rapidly at first, then it slows down as it becomes harder to select unused coordinates. This is basically the *coupon collectors* problem. The usual formulation of the coupon collectors problem has  $N$  different types of coupons or prizes in a cereal box. On each draw, one gets a coupon or prize equally likely to be any one of the  $N$  types. The goal is to find the expected number of coupons one needs to gather before getting a complete set of at least one of each type.

**Proposition 20.29.** *Sample uniformly with replacement from the set  $\{1, 2, \dots, N\}$ . Let  $\tau$  be the number of draws required until each element has been drawn at least once. Then*

$$\mathbb{E}[\tau] = N \sum_{\nu=0}^{N-1} \frac{1}{\nu+1}.$$

**Proof.** (1) The expectation  $\mathbb{E}[\tau]$  can be computed by writing  $\tau$  as a sum of geometric random variables.

(2) Let  $\tau_0 = 0$ . Let  $\tau_k$  be the number of selections when the collection first contains  $k$  distinct set elements.

(3) Then  $\tau = \tau_N = (\tau_1 - \tau_0) + (\tau_2 - \tau_1) + \dots + (\tau_N - \tau_{N-1})$ .

(4) Furthermore,  $\tau_k - \tau_{k-1}$  is a geometric random variable with success probability  $(N - k + 1)/N$ : after collecting  $k - 1$  coupons, there are  $N - k + 1$  types missing from the collection. Each subsequent coupon drawn has the same probability  $(N - k + 1)/N$  of being a type not already collected, until a new type is finally drawn.

(5) Thus

$$\mathbb{E}[\tau_k - \tau_{k-1}] = N/(N - k + 1).$$

(6)

$$\mathbb{E}[\tau] = \sum_{k=1}^N \mathbb{E}[\tau_k - \tau_{k-1}] = N \sum_{k=1}^N \frac{1}{N - k + 1} = N \sum_{\nu=0}^N \frac{1}{\nu}.$$

□

**Remark 20.30.** Recall that

$$\left| \sum_{\nu=1}^N \frac{1}{\nu} - \log N \right| \leq 1$$

so  $|\mathbb{E}[\tau] - N \log N| \leq N$ . (In fact,

$$\lim_{N \rightarrow \infty} \left( \sum_{\nu=1}^N \frac{1}{\nu} - \log N \right) = \gamma \approx 0.57721,$$

the Euler-Mascheroni constant. The estimate can be improved by using Stirling's approximation.)

But more about  $\tau$  can be said, the following lemma says  $\tau$  is unlikely to be much larger than the expected value.**Lemma 20.31.** *Sample uniformly with replacement from the set  $\{1, 2, \dots, N\}$ . Let  $\tau$  be the number of draws required until each element has been drawn at least once. Then*

$$\mathbb{P}[\tau > N \log N + cN] \leq e^{-c}$$

for  $c \geq 0$  and  $N \geq 1$ .**Proof.** Let  $m = N \log N + cN$ . For each integer  $\nu$  let  $A_\nu^{(m)}$  be the event “integer  $\nu$  not drawn in the first  $m$  draws”. Then

$$\mathbb{P}[\tau > m] = \mathbb{P}\left[\bigcup_{\nu=1}^N A_\nu^{(m)}\right] \leq \sum_{\nu=1}^N \mathbb{P}[A_\nu^{(m)}] = N \left(1 - \frac{1}{N}\right)^m \leq N e^{-m/N} = e^{-c}.$$

See the exercises for a proof of the second inequality. □

**Corollary 20.32.**

$$t(\epsilon) \leq N \log N + \log(\epsilon^{-1})N.$$

**Proof.** (1) Given  $\epsilon > 0$ ,  $t(\epsilon)$  is the smallest time  $t$  such that

$$\|\text{dist}(X_t) - \pi\|_{TV} < \epsilon.$$

(2) But

$$\|\text{dist}(X_t) - \pi\|_{TV} < \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - \pi\|_{TV} = d(t) \leq \bar{d}(t).$$

(3) A previous theorem gives a bound on  $\bar{d}(t)$  in terms of  $\mathbb{P}_{x,y}[\tau_{\text{coal}} > t]$ .(4) However,  $\tau_{\text{coal}}$  is the number  $\tau$  of draws required until each element has been drawn at least once. Then

$$\mathbb{P}[\tau > N \log N + cN] \leq e^{-c}.$$

- (5) So given  $\epsilon > 0$ , solving  $\epsilon = e^{-c}$  for  $c$  with  $c = \log(\epsilon^{-1})$ , the least time must be at least as great as  $N \log N + \log(\epsilon^{-1})N$ .

□

**Remark 20.33.** This upper bound uses a simple and natural coupling of the two lazy random walks started far apart. The next more sophisticated coupling of the two random walks gives an improved bound that justifies the information in Figure 20.6.

**Theorem 20.34.** *For the lazy random walk on the hypercube  $\mathbf{Q}^N$*

$$t(\epsilon) \leq \frac{1}{2}N \log N + \log(\epsilon^{-1})N.$$

- Proof.** (1) Let  $X_t = (X_t^1, \dots, X_t^N)$  be the position of the lazy random walk on  $\mathbf{Q}^N$ . Let  $W_t = ht(X_t) = \sum_{\nu=1}^N X_t^\nu$  be the Hamming weight of  $X_t$ .  
 (2) Note that  $W_t$  is the same as the alternate Ehrenfest model and recall that the stationary distribution for the alternate Ehrenfest model is  $\pi_W = \text{Bin}(N, 1/2)$ , the binomial distribution with parameters  $N$  and  $1/2$ .  
 (3) Claim:

$$\|\mathbb{P}_1[X_t] - \pi\|_{TV} = \|\mathbb{P}_n[W_t] - \pi_W\|_{TV}.$$

Proof of Claim: Let  $L_w$  be the level set of  $ht(x)$  on  $\mathbf{Q}^N$  corresponding to level  $w$ . The functions  $x \mapsto \mathbb{P}_1[X_t = x]$  and  $\pi$  are constant on  $L_w$ . Therefore

$$\sum_{x \in L_w} |\mathbb{P}_1[X_t = x] - \pi(x)| = \left| \sum_{x \in L_w} \mathbb{P}_1[X_t = x] - \pi(x) \right|$$

because all summands are equal. Then

$$\left| \sum_{x \in L_w} \mathbb{P}_1[X_t = x] - \pi(x) \right| = |\mathbb{P}_n[W_t = w] - \pi_W(w)|.$$

Summing over  $w = 0, 1, \dots, N$  and dividing by 2 gives the total variation metric, proving the claim.

- (4) Now construct a coupling  $(W_t, Z_t)$  of the alternate Ehrenfest chain started from  $w$  with the alternate Ehrenfest chain started from  $z$ . Provided that the two particles have not yet collided, at each move, a fair coin is tossed to determine which of the two particles moves; the chosen particle makes a transition according to the transition probability matrix of the alternate Ehrenfest model, while the other particle remains in its current position. The particles move together once they have met for the first time.  
 (5) Suppose, without loss of generality, that  $z \geq w$ . By the construction of the coupling, since the particles can't cross before they have met and are the same after they have met,  $Z_t \geq W_t$  for all  $t$ . Consequently, if  $D_t = |Z_t - W_t|$ , then  $D_t = Z_t - W_t \geq 0$ .

- (6) Let  $\tau_{textcoal} = \min \{t \geq 0 : Z_t = W_t\}$ . Conditioning on the event  $(Z_t, W_t) = (z_t, w_t)$  with  $z_t \neq w_t$ ,

$$D_{t+1} - D_t = \begin{cases} 1 & \text{with probability } (1/2)(1 - z_t/N) + (1/2)w_t/N \\ -1 & \text{with probability } (1/2)z_t/N + (1/2)(1 - w_t/N). \end{cases}$$

- (7) From the previous step, on the event  $\{\tau > t\}$ ,

$$\mathbb{E}_{z,w} [D_{t+1} - D_t \mid Z_t = z_t, W_t = w_t] = -\frac{z_t - w_t}{N} = -\frac{D_t}{N}.$$

- (8) Since  $\mathbf{1}_{\tau > t} = \mathbf{1}_{Z_t \neq W_t}$ ,

$$\mathbb{E}_{z,w} [\mathbf{1}_{\tau > t} D_{t+1} \mid Z_t, W_t] = \left(1 - \frac{1}{N}\right) D_t \mathbf{1}_{\tau > t}.$$

- (9) Taking expectation,

$$\mathbb{E}_{z,w} [D_{t+1} \mathbf{1}_{\tau > t}] = \left(1 - \frac{1}{N}\right) \mathbb{E}_{z,w} [D_t \mathbf{1}_{\tau > t}].$$

- (10) Since  $\mathbf{1}_{\tau > t+1} \leq \mathbf{1}_{\tau > t}$ ,

$$\mathbb{E}_{z,w} [D_{t+1} \mathbf{1}_{\tau > t+1}] \leq \left(1 - \frac{1}{n}\right) \mathbb{E}_{z,w} [D_t \mathbf{1}_{\tau > t}].$$

- (11) By induction

$$\mathbb{E}_{z,w} [D_{t+1} \mathbf{1}_{\tau > t}] \leq \left(1 - \frac{1}{N}\right)^t (z - w) \leq N e^{-t/N}.$$

- (12) From step 6, provided  $t < \tau$ , the process  $D_t$  is as least as likely to move up as it is to move down. Thus, until time  $\tau$ , the process  $D_t$  can be coupled with a simple random walk,  $S_t$ , so that  $S_0 = D_0$  and  $D_t \leq S_t$ .

- (13) If  $\bar{\tau} = \min \{t \geq 0 : S_t = 0\}$ , then  $\tau \leq \bar{\tau}$ .

- (14) There is a constant  $c_1$  such that  $k \geq 0$ ,

$$\mathbb{P}_k [\tau > u] \leq \mathbb{P}_k [\bar{\tau} > u] \leq \frac{c_1 k}{\sqrt{u}}.$$

- (15) Then

$$\mathbb{P}_{z,w} [\tau > s + u \mid D_s] = \mathbf{1}_{\tau > s} \mathbb{P}_{D_s} [\tau > u] \leq \frac{c_1 D_s \mathbf{1}_{\tau > s}}{\sqrt{u}}.$$

- (16) Taking expectation, and applying the inequality from the induction

$$\mathbb{P}_{z,w} [\tau > s + u] \leq \frac{c_1 n e^{-s/n}}{\sqrt{u}}.$$

- (17) Letting  $u = \alpha N$ , and  $s = (1/2)N \log N$

$$d_n((1/2)N \log N + \alpha N) \leq \frac{c_1}{\sqrt{\alpha}}.$$

- (18) Finally,

$$\lim_{\alpha \rightarrow \infty} \limsup_{n \rightarrow \infty} d_n((1/2)N \log N + \alpha N) = 0.$$

□

Next is a lower bound, which together with the upper bound gives tight estimates on the convergence to the stationary distribution.

**Theorem 20.35.** *Let  $\epsilon > 0$ . Then there exists an  $\alpha \geq 0$  so that for  $t(\alpha) = \frac{n}{2} \log n + \alpha n$ ,  $\mathbb{P}[\tau > t(\alpha)] < \epsilon$ .*

**Lemma 20.36.** (1) *Consider the coupon collecting problem with  $N$  distinct coupon types.*

(2) *Let  $I_j(t)$  be the indicator of the event that the  $j$ -th coupon has not been collected by time  $n$ .*

(3) *Let  $R_n = \sum_{j=1}^N I_j(n)$  be the number of coupon types not collected by time  $n$ .*

*Then the random variables  $I_j(n)$  are negatively correlated, and letting  $p = (1 - 1/N)^n$  for  $n \geq 0$ ,*

$$\mathbb{E}[R_n] = Np$$

$$\text{Var}[R_n] = Np(1 - p) \leq \frac{N}{4}.$$

**Remark 20.37.** With this notation, notice the similarity to the mean and variance of a binomial random variable. It helps to remember that  $N$  is the number of dimensions for the hypercube, and therefore the number of nonzero Hamming weights or hyperplane levels for the hypercube and the number of coupons in the collector's problem. The parameter  $n$  corresponds to the step of the Markov chain or random walk on the hypercube, and to the number of trials in the coupon collector's problem.

**Proof.** (1) Since  $I_j(n) = 1$  if and only if the first  $n$  coupons are not of type  $j$ , immediately

$$\mathbb{E}[I_j(n)] = \left(1 - \frac{1}{N}\right)^n = p$$

$$\text{Var}[I_j(n)] = p(1 - p).$$

(2) Similarly, for  $j \neq k$ ,

$$\mathbb{E}[I_j(n)I_k(n)] = \left(1 - \frac{2}{N}\right)^n.$$

(3) Therefore

$$\text{Cov}[I_j(n)I_k(n)] = \left(1 - \frac{2}{N}\right)^n - \left(1 - \frac{1}{N}\right)^{2n}.$$

(4) To establish

$$\left(1 - \frac{2}{N}\right)^n - \left(1 - \frac{1}{N}\right)^{2n} \leq 0$$

use proof by induction. It is trivially true for  $n = 0$ . Assuming that

$$\left(1 - \frac{2}{N}\right)^n - \left(1 - \frac{1}{n}\right)^{2n} \leq 0$$

and using the simple fact that

$$\left(1 - \frac{2}{N}\right) \leq \left(1 - \frac{1}{n}\right)^2$$

it follows that

$$\begin{aligned} \left(1 - \frac{2}{N}\right)^{n+1} &\leq \left(1 - \frac{1}{N}\right)^{2n} \left(1 - \frac{2}{N}\right) \\ &\leq \left(1 - \frac{1}{N}\right)^{2n} \left(1 - \frac{2}{N}\right)^2 = \left(1 - \frac{1}{N}\right)^{2(n+1)} \end{aligned}$$

□

**Definition 20.38.** When  $\mu$  is a probability distribution on  $\mathcal{X}$ , and  $f : \mathcal{X} \rightarrow \Lambda$  is a function on  $\mathcal{X}$ , write  $\mu f^{-1}$  for the probability distribution defined by

$$(\mu f^{-1})(A) = \mu(f^{-1}(A))$$

for  $A \subset \Lambda$ . When  $X$  is an  $\mathcal{X}$ -valued random variable with distribution  $\mu$ , then  $f(X)$  has distribution  $\mu f^{-1}$  on  $\Lambda$ .  $\diamond$

**Lemma 20.39.** (1) Let  $\mu$  and  $\nu$  be probability distributions on  $\mathcal{X}$ .

(2) Let  $f : \mathcal{X} \rightarrow \Lambda$  be a function on  $\mathcal{X}$  where  $\Lambda$  is a finite set.

Then  $\|\mu - \nu\|_{TV} \geq \|\mu f^{-1} - \nu f^{-1}\|_{TV}$ .

**Proof.** (1) First (read the parentheses carefully)

$$|\mu f^{-1}(B) - \nu f^{-1}(B)| = |\mu(f^{-1}(B)) - \nu(f^{-1}(B))|.$$

(2) Then

$$\max_{B \subset \Lambda} |\mu f^{-1}(B) - \nu f^{-1}(B)| \leq \max_{A \subset \mathcal{X}} |\mu(A) - \nu(A)|.$$

(3) The conclusion follows from the definition of the Total Variation metric.  $\square$

**Remark 20.40.** Use this lemma to lower bound the distance of some chain from stationarity in terms of the corresponding distance for a projection or lumping of that chain. To do so, take  $\Lambda$  to be the relevant partition of  $X$ .

**Proposition 20.41.** (1) Let  $f : \mathcal{X} \rightarrow \mathbb{R}$ .

(2) Let  $\mu, \nu$  be two probability distributions on  $\mathcal{X}$ .

(3) The notation  $\mathbb{E}_\mu[f]$  denotes the expectation of  $f(X)$  with respect to the measure  $\mu$ . Similarly for  $\mathbb{E}_\nu[f]$ ,  $\text{Var}_\mu[f]$ ,  $\text{Var}_\nu[f]$ .

(4) Define  $\sigma_\star^2 = \max[\text{Var}_\mu[f], \text{Var}_\nu[f]]$ .

(5) Suppose  $|\mathbb{E}_\mu[f] - \mathbb{E}_\nu[f]| \geq r\sigma_\star$ .

Then

$$\|\mu - \nu\|_{TV} \geq 1 - \frac{8}{r^2}.$$

**Proof.** (1) Suppose without loss of generality that  $\mathbb{E}_\mu[f] \leq \mathbb{E}_\nu[f]$ .

(2) Let  $A = (\mathbb{E}_\mu[f] + r\sigma_\star/2, \infty)$ , then Chebyshev's Inequality yields  $\mu f^{-1}(A) \leq \frac{4}{r^2}$  and  $\nu f^{-1}(A) \geq 1 - \frac{4}{r^2}$ .

(3) Then

$$\|\mu f^{-1} - \nu f^{-1}\|_{TV} \geq 1 - \frac{8}{r^2}.$$

(4) Then apply Lemma 20.39 to complete the proof.  $\square$

**Corollary 20.42.** *Suppose For a Markov chain  $X_t$  with transition probability matrix  $P$ , the function  $f$  satisfies*

$$|\mathbb{E}_x[f(X_t)] - \mathbb{E}_\pi[f]| \geq r\sigma_*$$

then

$$\|P^t(x, \cdot) - \pi\|_{TV} \geq 1 - \frac{8}{r^2}.$$

**Proof.** (1) See the exercises.  $\square$

**Proposition 20.43.** *For the lazy random walk on the  $N$ -dimensional hypercube*

$$d\left(\frac{1}{2}N \log N - \alpha N\right) \geq 1 - 8^{2-2\alpha}.$$

**Proof.** (1) Apply Proposition ?? with  $f = \text{ht}$ . That is, let  $W_n = \text{ht}(X_n)$  where the walker started at  $\bar{1}$  is  $X_n$ .

(2) As  $\pi$  is uniform on  $0, 1^N$ , the distribution of the random variable  $W$  is  $\text{Bin}(n, 1/2)$ , so  $\mathbb{E}_\pi[W] = n/2$  and  $\text{Var}_x[W] = n/4$ .

(3) Recall that  $R_n$  is the number of coordinates not updated by time  $t$ . When starting from  $\bar{1}$ , the conditional distribution of  $\text{ht}(X_n)$ , given  $R_n = r$  is  $r + \text{Bin}(n - r, 1/2)$ .

(4) Consequently,

$$\mathbb{E}_{\bar{1}}[\text{ht}(X_t) \mid R_n] = R_n + \frac{(n - R_n)}{2} = \frac{1}{2}(R_n + n).$$

(5) Using Lemma 20.36

$$\mathbb{E}_{\bar{1}}[\text{ht}(X_n)] = \frac{N}{2} \left[ 1 + \left(1 - \frac{1}{N}\right)^n \right].$$

(6) Recall the identity for variance using conditionals, applied here as

$$\begin{aligned} \text{Var}_{\bar{1}}[\text{ht}(X_n)] &= \text{Var}_{\bar{1}}[\mathbb{E}[\text{ht}(X_n) \mid R_n]] + \mathbb{E}_{\bar{1}}[\text{Var}_{\bar{1}}[\text{ht}(X_n) \mid R_n]] \\ &= \frac{1}{4} \text{Var}_{\bar{1}}[\text{ht}(X_n)] + \frac{1}{4} [N - \mathbb{E}_{\bar{1}}[R_n]]. \end{aligned}$$

(7) Again using Lemma 20.36,  $R_n$  is the sum of negatively correlated indicator functions and consequently,  $\text{Var}_{\bar{1}}[R_n] \leq \mathbb{E}_{\bar{1}}[R_n]$  so  $\text{Var}_{\bar{1}}[R_n] \leq N/4$ .

(8) Set

$$\sigma = \sqrt{\max[\text{Var}_\pi[W], \text{Var}_{\bar{1}}[\text{ht}(X_n)]]} = \frac{\sqrt{N}}{2}.$$

(9) Then

$$|\mathbb{E}_\pi[W] - \mathbb{E}_{\bar{1}}[\text{ht}(X_n)]| = \frac{N}{2} \left(1 - \frac{1}{N}\right)^n = \sigma \sqrt{N} \left(1 - \frac{1}{N}\right)^n.$$

(10) Set  $t_N = \frac{1}{2}(N-1)\log N - (\alpha-1)N > \frac{1}{2}N\log N - \alpha N$  and using  $(1-1/N)^{N-1} > e^{-1} > (1-1/N)^N$ ,

$$|\mathbb{E}_\pi[W] - \mathbb{E}_{\bar{1}}[\text{ht}(X_n)]| e^{\alpha-1} \sigma.$$

(11) Applying Lemma ?? gives

$$d\left(\frac{1}{2}N\log N - \alpha N\right) \geq \|P^{t_N}(\bar{1}, \cdot) - \pi\|_{TV} \geq 1 - 8e^{2-2\alpha}.$$

□

## 20.9. Chapter Ending Answer

For card players, shuffling the deck to remove any order is essential so that cards dealt from the deck come “at random”, that is, in an order uniformly distributed over all possible deck orders. For the Top-to-Random-Shuffle 7 shuffles of the 3-card deck gets close to the uniform density, which turns out to be the stationary density. With a riffle shuffle on a standard deck, 7 shuffles gets close to the uniform density.

## 20.10. Chapter Summary

### Key Concepts.

- (1) Card deck shuffles are a family of possible re-orderings with probability distributions, leading to transition probabilities, and thus Markov processes. The most well-studied type of shuffle is the riffle shuffle and that is the main focus here.
- (2) Going from card order  $\pi$  to  $\sigma$  is the same as composing  $\pi$  with the permutation  $\pi^{-1} \circ \sigma$ . Now identify shuffles as functions on  $\{1, \dots, n\}$  to  $\{1, \dots, n\}$ , that is, permutations. Since a particular shuffle is one of a whole family of shuffles, chosen with a probability distribution  $Q$  from the family, the transition probabilities are

$$p_{\pi\sigma} = \mathbb{P}[X_{t+1} = \sigma \mid X_t = \pi] = Q(\pi^{-1} \circ \sigma).$$

- (3) The identification of shuffles or operations with permutations gives a probability distribution on  $S_D$ .
- (4) A **Top-to-Random-Shuffle**, takes the top card from a stack of  $n$  cards and inserts it in the gap between the  $(\ell-1)$ th card and the  $\ell$ th card in the deck, where  $\ell$  is chosen randomly.
- (5) The Top-To-Random-Shuffle demonstrates the cut-off phenomenon for the Total Variation distance of the Markov chain distribution from the uniform distribution as a function of the number of steps.
- (6) One realistic model of shuffling a deck of cards is the **riffle shuffle**.



- (7) The set of cuts and interleavings in a riffle shuffle induces in a natural way a density on the set of permutations. Call this a **riffle shuffle** and denote it by  $R$ . That is,  $R(\pi)$  is the sum of probabilities of each cut and interleaving that gives the rearrangement of the deck corresponding to  $\pi$ .
- (8) 7 shuffles the of 3-card deck gets very close to the uniform density, which turns out to be the stationary density.
- (9) The probability of achieving a permutation  $\pi$  when doing an  $a$ -shuffle is

$$\frac{1}{a^n} \binom{n+a-r}{n},$$

where  $r$  is the number of rising sequences in  $\pi$ .

- (10) The eigenvalues of the transition probability matrix for a riffle shuffle are  $1, \frac{1}{2}, \frac{1}{4}$  and  $\frac{1}{2^n}$ . The second largest eigenvalue determines the rate of convergence to the stationary distribution. For riffle shuffling, this eigenvalue is  $\frac{1}{2}$ .
- (11) For a finite, irreducible, aperiodic Markov chain  $Y_t$  distributed as  $Q^t$  at time  $t$  and with stationary distribution  $\pi$ , and  $\tau$  is a strong stationary time, then

$$\|Q^\tau - \pi\|_{TV} \leq \mathbb{P}([\tau \geq t]).$$

- (12) Set  $d_n(t) = \|P^{\tau_{\text{top}}+1} - U\|_{TV}$ . Then for  $\epsilon > 0$ ,
- (a)  $d_n(n \log n + n \log \epsilon^{-1}) \leq \epsilon$  for  $n$  sufficiently large.
  - (b)  $d_n(n \log n - n \log(C\epsilon^{-1})) \geq 1 - \epsilon$  for  $n$  sufficiently large.

### Vocabulary.

- (1) A **Top-to-Random-Shuffle**, takes the top card from a stack of  $n$  cards and inserts it in the gap between the  $(k-1)$ th card and the  $k$ th card in the deck.
- (2) The **total variation distance** of  $\mu$  from  $\nu$  is

$$\|\mu - \nu\|_{TV} = \max_{A \subset \Omega} |\mu(A) - \nu(A)| = \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|.$$

- (3) A stopping time  $\tau_{\text{top}}$  is a **strong stationary time** for  $X_t$ ,  $t \geq 0$  if  $X_{\tau_{\text{top}}+1} \sim \text{unif}(S_n)$ , and  $X_{\tau_{\text{top}}+1}$  is independent of  $\tau_{\text{top}}$ .
- (4) The **riffle shuffle** first cuts the deck randomly into two packets, one containing  $k$  cards and the other containing  $n-k$  cards. Choose  $k$ , the number of cards cut according to the binomial density. Once the deck is cut into two packets, interleave the cards from each packet in any possible way, such that the cards from each packet keep their own relative order.
- (5) A special case of the riffle shuffle is the **perfect shuffle**, also known as the **faro shuffle** wherein the two packets are completely interleaved.
- (6) A **rising sequence** of a permutation is a maximal consecutive increasing subsequence.
- (7) A  **$a$ -shuffle** is another probability density on  $S_n$ . Let  $a$  be any positive integer. Cut the deck into  $a$  packets of nonnegative sizes  $m_1, m_2, \dots, m_a$  with  $m_1 + \dots + m_a = n$  but some of the  $n_i$  may be zero. Interleave the cards from each packet in any way, so long as the cards from each packet keep the relative order

among themselves. With a fixed packet structure, consider all interleavings equally likely.

**Notation.**

- (1)  $S_n$  – The set of states for a Markov process modeling the order of the deck, the set of permutations on  $n$  cards.
- (2) Initial state  $X_0$  – the identity permutation with probability 1
- (3)  $\pi$  and  $\sigma$  – particular card orders
- (4) probability distribution  $Q$  from the family of shuffles, the transition probabilities are  $p_{\pi\sigma} = \mathbb{P}[X_{t+1} = \sigma \mid X_t = \pi] = Q(\pi^{-1} \circ \sigma)$ .
- (5)  $P$  – transition probability matrix
- (6)  $t$  – epoch or time for the Markov chain
- (7)  $k$  – arbitrary card or position in deck of  $n$  cards
- (8)  $U$  – uniform distribution on a group, or more generally a state space
- (9)  $Q$  be a probability distribution on a finite group  $G$  inducing an irreducible and aperiodic Markov chain with transition probabilities  $Q(\pi^{-1} \circ \sigma)$  from  $\pi$  to  $\sigma$
- (10)  $\tau_{\text{top}}$  be the first time that card  $n$  reaches the top of the deck
- (11) If  $\mu$  and  $\nu$  are probability distributions on  $\Omega$ , the **total variation distance** of  $\mu$  from  $\nu$  is  $\|\mu - \nu\|_{TV}$
- (12)  $V$  – the number of draws required until each ball has been drawn at least once
- (13) set  $d_P(n) = \|P^n - U\|_{TV}$
- (14)  $\tau_i$  – the time until card  $i$  is placed under the original bottom card
- (15)  $V_i$  – the number of draws required until  $i$  distinct balls have been drawn at least once
- (16)  $A_j$  – the set of configurations of the deck such that the bottom  $j$  original cards stay in their original relative order. Plainly  $U(A_j) = \frac{1}{j!}$
- (17)  $k = k(n) = n \log n - c_n n$  where  $c_n \rightarrow \infty$
- (18) cut the deck randomly into two packets, one containing  $k$  cards and the other containing  $n - k$  cards. Choose the number of cards cut,  $k$ , according to the binomial density
- (19) Call the density a *riffle shuffle* and denote it by  $R$ . That is,  $R(\pi)$  is the sum of probabilities of each cut and interleaving that gives the rearrangement of the deck corresponding to  $\pi$
- (20)  $a$  – number of packets of nonnegative sizes  $m_1, m_2, \dots, m_a$  with  $m_1 + \dots + m_a = n$  but some of the  $m_i$  may be zero
- (21)  $R_a$  – induced density on the permutations leading to the cuts and shuffles is then called the  $a$ -shuffle with notation



## Coupling and Minorization

This section considers convergence rates for Markov chains. It is already clear why knowing the convergence rates are important for MCMC algorithms. Already introduced is the eigenvalue method. This section introduces the coupling method, and minorization and drift conditions, and applies them to examples on state spaces ranging from finite to compact to unbounded.

Bounding a Markov chain's convergence rate is not a one-time, definitive process; for various Markov chains, it is possible to strengthen the bound through careful and creative new constructions. The bounds presented in this section all have their imperfections, and will certainly not give tight or realistic bounds for all examples. Nevertheless the estimates permit running MCMC algorithms more confidently and reliably.

Rating: Mathematicians Only: prolonged scenes of intense rigor.

### 21.1. Chapter Starter Question

In the Chapter on Fundamental Theorems for Markov Chains, the proof of the Convergence Theorem by Total Variation relies on what estimate for all entries in the transition probability matrix?

### 21.2. Coupling and Minorization Definitions

The idea of coupling is to create two different copies of a random object, and compare them. Coupling has a long history in probability theory, with many different applications and approaches. A key idea is the following simple lemma.

**Lemma 21.1** (Coupling Inequality). *Let  $X$  and  $Y$  be 2 random variables, each with its own distribution. Then for any event  $A$*

$$|\mathbb{P}[X \in A] - \mathbb{P}[Y \in A]| \leq \mathbb{P}[X \neq Y].$$

**Proof.** (1) First

$$|\mathbb{P}[X \in A] - \mathbb{P}[Y \in A]| = |\mathbb{P}[X \in A, X = Y] + \mathbb{P}[X \in A, X \neq Y] - \mathbb{P}[Y \in A, X = Y] - \mathbb{P}[Y \in A, X \neq Y]|.$$

(2) But  $\mathbb{P}[X \in A, X = Y] = \mathbb{P}[Y \in A, X = Y]$  since both are the same event, so the two terms cancel.

(3) Since  $0 \leq \mathbb{P}[X \in A, X \neq Y] \leq \mathbb{P}[X \neq Y]$  and  $0 \leq \mathbb{P}[Y \in A, X \neq Y] \leq \mathbb{P}[X \neq Y]$ , the difference of the two probabilities must be less or equal to  $\mathbb{P}[X \neq Y]$ .

(4) In summary

$$|\mathbb{P}[X \in A] - \mathbb{P}[Y \in A]| \leq \mathbb{P}[X \neq Y].$$

□

Recall  $\text{dist}(X)$  is the probability distribution for  $X$ . Also recall the definition of the total variation distance.

**Corollary 21.2.**

$$\|\text{dist}(X) - \text{dist}(Y)\|_{TV} \leq \mathbb{P}[X \neq Y].$$

**Proof.** Since the upper bound in the coupling inequality is uniform over subsets  $A$ , take the supremum over  $A$ . □

**Definition 21.3.** A Markov chain with state space  $\mathcal{X}$  and transition probabilities  $P$  satisfies a **minorization condition** if there exists a measurable subset  $C \subset \mathcal{X}$ , a probability measure  $\mu$  on  $\mathcal{X}$ , a constant  $\epsilon > 0$ , and a positive integer  $n_0$ , such that

$$P^{n_0}(x, \cdot) \geq \epsilon \mu(\cdot), x \in C.$$

Such a set  $C$  satisfying the minorization condition is a **small set**. In particular, if  $C = \mathcal{X}$  (the entire state space), then the Markov chain satisfies a **uniform minorization condition**, also referred to as *Doebelin's condition*. ◇

**Example 21.4.** For an example, suppose the state space is the half-line  $\mathcal{X} = [0, \infty)$ , with transition probabilities given by

$$P(x, dy) = \left( e^{-2y} + \frac{1}{\sqrt{2\pi}(x+1)} e^{-\frac{y^2}{2(x+1)^2}} \right) dy.$$

That is, from a state  $x$ , the chain moves to an equal mixture of an Exponential(2) distribution and a half-normal distribution with mean 0 and standard deviation  $x+1$ . In this case,  $P(x, dy) \geq e^{-2y} dy$  for all  $x$ , so the chain satisfies a uniform minorization condition with  $n_0 = 1$ ,  $\mu(y) = 2e^{-2y}$ , and  $\epsilon = 1$ . ▽

The uniform minorization condition implies that there exists a common overlap of size  $\epsilon$  between all of the transition probabilities. This allows a coupling construction of two different copies  $X_n$  and  $X'_n$  of a Markov chain, as follows. Assume for now that  $n_0 = 1$ . First, choose  $X_0 \sim \mu_0(\cdot)$  and  $X'_0 \sim \pi(\cdot)$  independently. Then, inductively for  $n = 0, 1, 2, \dots$ :

- (1) If  $X_n = X'_n$ , choose  $z \sim P(X_n, \cdot)$  and let  $X_{n+1} = X'_{n+1} = z$ . The chains have already coupled, and they will remain equal forever.

- (2) If  $X_n \neq X'_n$ , flip a coin whose probability of Heads is  $\epsilon$ . If the coin shows Heads, choose  $z \sim \mu(\cdot)$  and let  $X_{n+1} = X'_{n+1} = z$ . Otherwise, update  $X_{n+1}$  and  $X'_{n+1}$  independently with

$$\begin{aligned}\mathbb{P}[X_{n+1} \in A] &= \frac{P(X_n, A) - \epsilon\mu(A)}{1 - \epsilon}, \\ \mathbb{P}[X'_{n+1} \in A] &= \frac{P(X'_n, A) - \epsilon\mu(A)}{1 - \epsilon}.\end{aligned}$$

The minorization condition guarantees that these probabilities are nonnegative, and hence are probability measures since their total mass is

$$\frac{P(X_n, \mathcal{X}) - \epsilon\mu(\mathcal{X})}{1 - \epsilon} = \frac{1 - \epsilon}{1 - \epsilon} = 1.$$

The claim is that this construction ensures that overall,  $\mathbb{P}[X_{n+1} \in A \mid X_n = x] = P(x, A)$  and  $\mathbb{P}[X'_{n+1} \in A \mid X'_n = x] = P(x, A)$  for any  $x \in \mathcal{X}$ . To prove the claim, if the two chains are unequal at time  $n$ , then

$$\begin{aligned}\mathbb{P}[X_{n+1} \in A \mid X_n = x] &= \mathbb{P}[X_{n+1} \in A, \text{ Heads} \mid X_n = x] + \mathbb{P}[X_{n+1} \in A, \text{ Tails} \mid X_n = x] \\ &= \mathbb{P}[\text{ Heads}] \mathbb{P}[X_{n+1} \in A, \mid X_n = x, \text{ Heads}] + \mathbb{P}[\text{ Tails}] \mathbb{P}[X_{n+1} \in A, \mid X_n = x, \text{ Tails}] \\ &= \epsilon\mu(A) + (1 - \epsilon) \frac{P(X_n, A) - \epsilon\mu(A)}{1 - \epsilon} \\ &= P(x, A).\end{aligned}$$

If  $n_0 > 1$ , use the above construction for times  $n = 0, n_0, 2n_0, \dots$  with  $n + 1$  replaced by  $n + n_0$ , and with  $P(\cdot, \cdot)$  replaced by  $P^{n_0}(\cdot, \cdot)$ . Then, if desired, later “fill in” the intermediate states  $X_n$  for  $jn_0 < n < (j + 1)n_0$  from their appropriate conditional distributions given the already-constructed values of  $X_{jn_0}$  and  $X_{(j+1)n_0}$ .

Since  $X'_0 \sim \pi(\cdot)$  and  $\pi$  is a stationary distribution,  $X'_n \sim \pi(\cdot)$  for all  $n$ . Every  $n_0$  steps, the two chains’ probability is at least  $\epsilon$  of coupling, that is, of the coin showing Heads. So,  $\mathbb{P}([X_n \neq X'_n] \leq (1 - \epsilon)\lfloor n/n_0 \rfloor$ . The coupling equality then implies the following.

**Theorem 21.5** (Uniform Minorization Estimate). *If  $X_n$  is a Markov chain on  $\mathcal{X}$ , whose transition probabilities satisfy a uniform minorization condition for some  $\epsilon > 0$ , then for any positive integer  $n$  and any  $x \in \mathcal{X}$ ,*

$$\|\text{dist}(X_n) - \pi(\cdot)\|_{TV} \leq (1 - \epsilon)^{\lfloor n/n_0 \rfloor}.$$

**Example 21.6.** The previous example, with state space as the half-line  $\mathcal{X} = [0, \infty)$ , with transition probabilities given by

$$P(x, dy) = \left( e^{-2y} + \frac{1}{\sqrt{2\pi}(x+1)} e^{-\frac{y^2}{2(x+1)^2}} \right) dy$$

showed that  $n_0 = 1$ ,  $\mu(y) = 2e^{-2y}$ , and  $\epsilon = 1$ . The Theorem implies  $\|\text{dist}(X_n) - \pi(\cdot)\|_{TV} \leq (1 - \epsilon)^{\lfloor n/n_0 \rfloor} = (1/2)^n$  which is less than 0.01 if  $n \geq 6$ . That is, this chain converges to that degree of accuracy within six steps.  $\nabla$

**Corollary 21.7.** *If  $\mathcal{X}$  is finite, and for some  $n_0$  there is at least one state  $j \in \mathcal{X}$  such that the  $j$ th column of  $P^{n_0}$  is all positive, i.e.,  $(P^{n_0})_{ij} > 0$  for all  $i \in \mathcal{X}$ . Set  $\epsilon = \sum_{j \in \mathcal{X}} \min_{i \in \mathcal{X}} (P^{n_0})_{ij} > 0$ , and  $\mu(j) = \epsilon^{-1} \min_{i \in \mathcal{X}} (P^{n_0})_{ij}$ . Then an  $n_0$ -step uniform minorization condition is satisfied with  $\epsilon$ .*

**Proof.** Note that  $(P^{n_0})_{ij} \geq \epsilon \mu(j)$  for all  $i, j \in \mathcal{X}$ .  $\square$

**Example 21.8.** Consider the alternative Ehrenfest urn model. Two urns, labeled  $A$  and  $B$ , contain a total of  $N = 7$  balls. At each step a ball is selected at random with all selections equally likely. Then an urn is selected, urn  $A$  with probability  $p = \frac{1}{2}$  and urn  $B$  with probability  $q = 1 - p = \frac{1}{2}$  and the ball is moved to that urn. The state at each step is the number of balls in the urn  $A$ , from 0 to  $N$ . Let the state be the number of balls in urn  $A$ . The transition probability matrix is

$$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/14 & 1/2 & 3/7 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/7 & 1/2 & 5/14 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3/14 & 1/2 & 2/7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2/7 & 1/2 & 3/14 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5/14 & 1/2 & 1/7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3/7 & 1/2 & 1/14 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 \end{pmatrix}.$$

This Markov chain has a stationary distribution

$$\pi = (1/128, 7/128, 21/128, 35/128, 35/128, 21/128, 7/128, 1/128).$$

This Markov chain is ergodic and aperiodic. All states are accessible and all states communicate. This Markov chain has no transient states and all states are recurrent. This Markov chain has no absorbing states.

Following the proof,

$$P^4 = \begin{pmatrix} 0.11953 & 0.34694 & 0.3586 & 0.15306 & 0.02187 & 0.0 & 0.0 & 0.0 \\ 0.04956 & 0.22199 & 0.36297 & 0.26864 & 0.08746 & 0.00937 & 0.0 & 0.0 \\ 0.01708 & 0.12099 & 0.29654 & 0.33528 & 0.18326 & 0.04373 & 0.00312 & 0.0 \\ 0.00437 & 0.05373 & 0.20117 & 0.33569 & 0.27697 & 0.10995 & 0.01749 & 0.00062 \\ 0.00062 & 0.01749 & 0.10995 & 0.27697 & 0.33569 & 0.20117 & 0.05373 & 0.00437 \\ 0.0 & 0.00312 & 0.04373 & 0.18326 & 0.33528 & 0.29654 & 0.12099 & 0.01708 \\ 0.0 & 0.0 & 0.00937 & 0.08746 & 0.26864 & 0.36297 & 0.22199 & 0.04956 \\ 0.0 & 0.0 & 0.0 & 0.02187 & 0.15306 & 0.3586 & 0.34694 & 0.11953 \end{pmatrix}$$

has strictly positive entries in column 4 (state 3, and the symmetrical column 5, state 4) which is reasonable since there is at least a  $15/686$  chance of 4 transitions from state 0 to any state, including state 7. Note that  $\sum_{j \in \mathcal{X}} \min_{i \in \mathcal{X}} (P^{n_0})_{ij} = 0 + 0 + 0 + 15/686 + 15/686 + 0 + 0 + 0 + 30/686 > 0.043$ . For convenience take  $\epsilon = 0.043$  and  $\mu(j) = \epsilon^{-1} \min_{i \in \mathcal{X}} (P^{n_0})_{ij}$ . Then by the Theorem, the Total Variation distance to the stationary distribution is less than  $(1 - \epsilon)^{\lfloor n/4 \rfloor}$ . From any starting distribution, the Theorem says to have the total variation distance of the chain distribution to the stationary distribution less than 0.01, it is sufficient to make 105 steps. This is a much better estimate than the estimate from the proof of Convergence by Total Variation.

Since the second largest magnitude eigenvalue of  $P$  is approximately 0.85714, the eigenvalues suggest that it will take about  $\log(0.01)/\log(0.85714) \approx 29.874$  steps to make the total variation distance of the chain distribution to the stationary distribution less than 0.01. In fact, by numerical experimentation, it takes 31 steps to make the total variation distance from the stationary distribution less than 0.01, and even then only when starting from one of the extreme states 0 or 7.

▽

### 21.3. Pseudo-minorization Conditions

The coupling construction used to prove Theorem 21.5 was a pairwise construction, it only considered two chain locations  $x$  and  $y$  at a time. Replacing the distribution  $\mu(\cdot)$  with  $\mu_{xy}(\cdot)$ , allowing it to depend on  $x$  and  $y$ , then  $C$  is called a **pseudo-small set**, and Theorem 1 continues to hold ???. It then follows that on a finite state space, choosing

$$\epsilon = \min_{i,j \in \mathcal{X}} \sum_{z \in \mathcal{X}} \min\{(P^{n_0})_{iz}, (P^{n_0})_{jz}\} > 0$$

$$\mu_{ij}(Z) = \frac{\min\{(P^{n_0})_{iz}, (P^{n_0})_{jz}\}}{\sum_{w \in \mathcal{X}} \min\{(P^{n_0})_{iw}, (P^{n_0})_{jw}\}}$$

then the chain will satisfy an  $n_0$ -step pseudo-minorization condition, i.e., for all  $i, j, z \in \mathcal{X}$ ,  $(P^{n_0})_{iz} \geq \epsilon \mu_{ij}(z)$  and  $(P^{n_0})_{jz} \geq \epsilon \mu_{ij}(z)$ . Exactly as before,  $\|\text{dist}(X_n) - \pi(\cdot)\|_{TV} \leq (1 - \epsilon)^{\lfloor n/n_0 \rfloor}$ .

**Example 21.9.** Consider the alternate Ehrenfest urn model again. Once again,  $P^4$  has strictly positive entries in column 4. Then

$$\min_{i,j \in \mathcal{X}} \sum_{z \in \mathcal{X}} \min\{(P^{n_0})_{iz}, (P^{n_0})_{jz}\} \approx 0.044$$

occurring for state pair  $(i, j) = (0, 7)$  (or the symmetric state  $(7, 0)$ ) which makes sense since these states have the least overlap. The pseudo-minorization conditions do not yield a significant improvement in the estimate of convergence rates. ▽

### 21.4. Continuous State Space

The above analysis was primarily focused on finite state spaces. Now extend to continuous examples on subsets of  $\mathbb{R}^d$ . To be specific, consider a point process consisting of three particles each randomly located within the closed square  $[0, 1]^2 \subset \mathbb{R}^2$ , with positions denoted by  $x_i = (x_{i1}, x_{i2})$  for  $i = 1, 2, 3$ , so the state space  $\mathcal{X} = [0, 1]^6$ . Suppose these particles are distributed according to a probability distribution with unnormalized density (meaning that the actual density is a constant multiple of so it integrates to 1) given by

$$\pi(\mathbf{x}) = \pi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \exp \left( -C \sum_{\nu=1}^3 \|\mathbf{x}_\nu\| - D \sum_{i < j} \|\mathbf{x}_i - \mathbf{x}_j\|^{-1} \right)$$

where  $C$  and  $D$  are fixed positive constants, and  $\|\cdot\|$  is the usual Euclidean norm on  $\mathbb{R}^2$ . In this density, the first sum pushes the particles towards the origin, and the



second sum pushes them away from each other. Create a Markov chain which has  $\pi$  as its stationary distribution. To do this, use a version of the Metropolis Algorithm. Each step of the Markov chain proceeds as follows. Given  $X_n = \mathbf{x}$ , first “propose” to move the particles from their current configuration  $\mathbf{x}$  to some other configuration  $\mathbf{y}$ , chosen from the uniform (i.e., Lebesgue) measure on  $\mathcal{X}$ . Then, with probability  $\min[1, \frac{\pi(\mathbf{y})}{\pi(\mathbf{x})}]$ , “accept” this proposal and move to the new configuration by setting  $X_{n+1} = \mathbf{y}$ . Otherwise, “reject” this proposal and leave the configuration unchanged by setting  $X_{n+1} = \mathbf{x}$ . As in the chapter on the Metropolis Algorithm, this simple procedure creates a Markov chain which has  $\pi$  as its stationary distribution. As always, to get reliable samples, it is important to know how many iterations are required to approximately converge to  $\pi$ , i.e., to establish quantitative convergence bounds. The above Markov chain has an uncountably infinite state space  $\mathcal{X}$ , so eigenvalue analysis is not available. On the other hand, the uniform minorization condition can still be applied.

**Proposition 21.10.** *The Markov chain constructed above satisfies a uniform minorization condition with  $n_0 = 1$  and  $\epsilon = (0.48)e^{-C(4.25)-D(9.88)}$ .*

**Proof.** (1) To avoid problematic configurations where the particles are close together, set  $\mathcal{X}' = \{(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) : |\mathbf{x}_i - \mathbf{x}_j| \geq 1/4, 1 \leq i < j \leq 3\}$ .

(2)  $\mathcal{X}'$  is a compact set, and  $\pi$  is continuous and positive,  $\pi$  must achieve its minimum

$$m = \min_{\mathbf{x}, \mathbf{y}} \frac{\pi(\mathbf{y})}{\pi(\mathbf{x})} > 0$$

on  $\mathcal{X}'$ .

(3) Let  $A \subset \mathcal{X}$ . By the standard MCMC algorithm, the chain will move into  $A$  on the next step provided that the proposed new configuration  $\mathbf{y}$  is within the subset  $A$  and the proposal is accepted.

(4) That is

$$P(\mathbf{x}, A) = \int_A P(\mathbf{x}, d\mathbf{y}) = \int_A \min \left[ 1, \frac{\pi(\mathbf{y})}{\pi(\mathbf{x})} \right] d\mathbf{y} \geq \int_{A \cap \mathcal{X}'} m d\mathbf{y} = m \text{Leb}(A \cap \mathcal{X}')$$

where  $\text{Leb}()$  is Lebesgue measure on  $\mathbb{R}^6$ .

(5) So set  $\epsilon = m \text{Leb}(\mathcal{X}')$  and  $\mu(A) = \text{Leb}(A \cap \mathcal{X}') / \text{Leb}(\mathcal{X}')$ , then  $\epsilon > 0$  and  $P(x, A) \geq \epsilon \mu(A)$  so a uniform minorization condition is satisfied.

(6) To obtain quantitative convergence bounds requires estimation of  $\text{Leb}(\mathcal{X}')$ .

(7) For  $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \in \mathcal{X}'$ , first choose any  $\mathbf{x}_1 \in [0, 1]^2$  (which has two-dimensional area 1), then choose  $\mathbf{x}_2 \in [0, 1]^2 \setminus \text{Ball}(\mathbf{x}_1, 1/4)$  (which has two-dimensional area greater than  $1 - 3.14 \cdot (1/4)^2$ ), then choose  $\mathbf{x}_3 \in [0, 1]^2 \setminus (\text{Ball}(\mathbf{x}_1, 1/4) \cup \text{Ball}(\mathbf{x}_2, 1/4))$  (which has two-dimensional area greater than  $1 - 3.14 \cdot (1/4)^2 - 3.14 \cdot (1/4)^2$ ).

(8) Hence  $\text{Leb}(\mathcal{X}') > (1) \cdot (1 - \frac{3.14}{16}) \cdot (1 - \frac{3.14}{8}) \approx 0.488278125 \geq 0.48$ .

(9) Also for any  $\mathbf{x} \in \mathcal{X}'$ , it is the case that  $0 \leq |\mathbf{x}_i| \leq \sqrt{2}$  and  $1/4 \leq |\mathbf{x}_i - \mathbf{x}_j| \leq \sqrt{2}$  so

$$0 \leq |\mathbf{x}_1| + |\mathbf{x}_2| + |\mathbf{x}_3| \leq 3\sqrt{2}$$

and

$$\frac{3}{\sqrt{2}} \leq \sum_{i < j} |\mathbf{x}_i - \mathbf{x}_j| \leq 12.$$

(10) Then

$$m \geq \frac{e^{-C \cdot 3\sqrt{2} - D \cdot 12}}{e^{-C \cdot 0 - D \cdot 3/\sqrt{2}}} = e^{-C \cdot 3\sqrt{2} - D \cdot (12 - 3/\sqrt{2})} \geq e^{-C \cdot 4.25 - D \cdot 9.88}$$

since  $3\sqrt{2} \approx 4.24264$  and  $3/\sqrt{2} \approx 9.87868$ .

(11) Then  $\epsilon = m \text{Leb}(\mathcal{X}') \geq 0.48 \cdot e^{-C \cdot 4.25 - D \cdot 9.88}$ .

□

**Example 21.11.** If  $C = D = 1/10$ , then take  $\epsilon = 0.117$ . It then follows from Theorem 21.5 that we have the convergence bound  $\|\text{dist}(X_n) - \pi(\cdot)\|_{TV} \leq (1 - \epsilon)^n = (1 - 0.117)^n = (0.883)^n$ . This shows that after  $n = 38$  steps, the total variation distance between this continuous state space Markov chain and the stationary distribution will be less than 0.01. ▽

## 21.5. Unbounded State Space and Drift Conditions

In many cases, especially on unbounded state spaces, the minorization condition cannot be satisfied uniformly, only on some subset  $C \subset \mathcal{X}$ . In such cases, adjust the previous  $n_0 = 1$  coupling construction, as follows. First choose  $X_0 \sim \mu(\cdot)$  and  $X'_0 \sim \pi(\cdot)$  independently, and then inductively for  $n = 0, 1, 2, \dots$ :

- (1) If  $X = X'$ , choose  $X_{n+1} = X'_{n+1} \sim P(X, \cdot)$ .
- (2) Else, if  $(X_n, X'_n) \in C \times C$  flip a coin whose probability of Heads is  $\epsilon$ , and then update  $X_{n+1}$  and  $X'_{n+1}$  in the same way as in step 2 of the previous (uniform minorization) construction above.
- (3) Else, if  $(X_n, X'_n) \notin C \times C$ , then conditionally independently choose  $X_{n+1} \sim P(X_n, \cdot)$  and  $X'_{n+1} \sim P(X'_n, \cdot)$ , i.e., the two chains are simply updated independently.

The construction above provides good coupling bounds provided that the two chains return to  $C \times C$  often enough, but this last property is difficult to guarantee. Thus, to obtain convergence bounds also requires a drift condition. Basically, the drift condition guarantees that the chains will return to  $C \times C$  quickly enough to still achieve a coupling.

**Definition 21.12.** A Markov chain with a small set  $C \subset \mathcal{X}$  satisfies a **bivariate drift condition** if there exists a function

$$h : \mathcal{X} \times \mathcal{X} \rightarrow [1, \infty)$$

and some  $\alpha > 1$  such that

$$\bar{P}h(x, y) \leq h(x, y)/\alpha$$

where

$$\bar{P}h(x, y) := \mathbb{E}[h(X_{n+1}, Y_{n+1}) \mid X_n = x, Y_n = y]$$

is the expected or average value of  $h(x_{n+1}, y_{n+1})$  on the next iteration, when the chains start from  $x$  and  $y$  respectively and proceed independently. ◇

Such bivariate drift conditions can be combined with nonuniform minorization conditions to produce quantitative convergence bounds. To state them, use the quantity  $B_{n_0} = \max\{1, \alpha^{n_0}(1 - \epsilon) \sup_{C \times C} \bar{R}h\}$  where

$$\bar{R}h(x, y) = \int_{\mathcal{X}} \int_{\mathcal{X}} (1 - \epsilon)^{-2} h(z, w) [P^{n_0}(x, dz) - \epsilon \mu(dz)] [P^{n_0}(x, dw) - \epsilon \mu(dw)]$$

This daunting expression represents the expected value of  $h(X_{n+n_0}, X'_{n+n_0})$  given that  $X_n = x$ , that  $X'_n = y$ , and that the two chains fail to couple at time  $n$  (i.e., the corresponding coin shows Tails). In certain situations,  $\bar{R}h$  simplifies. For example, if  $D$  is a set such that  $P^{n_0}(x, D) = 1$  for all  $x \in C$ , then since the expected value of a random variable is always less than the maximal value it could take,

$$\sup_{(x,y) \in C \times C} \bar{R}h \leq \sup_{(x,y) \in D \times D} h(x, y).$$

**Theorem 21.13.** *Consider a Markov chain on  $\mathcal{X}$ , with  $X_0 = x$ , and transition probabilities  $P$ . Suppose the above minorization and bivariate drift conditions hold for some  $C \subset \mathcal{X}$ ,  $h : \mathcal{X} \times \mathcal{X} \rightarrow [1, \infty)$ , probability distribution  $\mu(\cdot)$ ,  $\alpha > 1$ , and  $\epsilon > 0$ . Then for any integers  $1 \leq j \leq n$ , with  $B_{n_0}$  as above,*

$$\|\text{dist}(X_n) - \pi(\cdot)\|_{TV} \leq (1 - \epsilon)^j + \alpha^{-n} B_{n_0}^{j-1} \mathbb{E}_{Z \sim \pi} [h(x, Z)].$$

**Proof.** (1) Create a second copy of the Markov chain with  $X'_0 \sim \pi$ , and use the above coupling construction.

(2) Let  $N_n$  be the number of times the chain  $(X_n, X'_n)$  is in  $C \times C$  by the  $n$ th step.

(3) By the coupling inequality

$$\|\text{dist}(X_n) - \pi(\cdot)\|_{TV} \leq \mathbb{P}[X_n \neq X'_n] \leq \mathbb{P}[X_n \neq X'_n, N_{n-1} \geq j] + \mathbb{P}[X_n \neq X'_n, N_{n-1} < j].$$

(4) The first term suggests that the chains have not coupled by time  $n$  despite visiting  $C \times C$  at least  $j$  times. Since each such time gives them a chance of  $\epsilon$  to couple, the first term is less than  $(1 - \epsilon)^j$ . The second term is more complicated, but from the bivariate drift condition together with a martingale argument, it can be shown to be no greater than  $\alpha^{-n} B_{n_0}^{j-1} \mathbb{E}_{Z \sim \pi} [h(x, Z)]$ .  $\square$

## 21.6. Drift Conditions

Sometimes it is hard to directly check the bivariate drift condition. This section introduces the more easily-verified univariate drift condition, and gives a way to derive the bivariate condition from the univariate one.

**Definition 21.14.** A Markov chain with a small set  $C$  satisfies a **univariate drift condition** if there are constants  $0 < \lambda < 1$  and  $b < \infty$ , and a function  $V : \mathcal{X} \rightarrow [1, \infty]$ , such that

$$PV(x) \leq \lambda V(x) + b \mathbf{1}_C(x), \quad x \in \mathcal{X}$$

where  $PV(x) = \mathbb{E}[V(X_n + 1) \mid X_n = x]$ .  $\diamond$

This univariate drift condition can be used to bound  $\mathbb{E}_\pi[V]$ . Indeed, assuming  $\mathbb{E}_\pi[V] < \infty$ , stationarity then implies that  $\mathbb{E}_\pi[V] \leq \mathbb{E}_\pi[V] + b$ , whence  $\mathbb{E}_\pi[V] \leq b/(1 - \text{lambda})$ . But also, univariate drift conditions can imply bivariate drift conditions, as follows.

**Proposition 21.15.** *Suppose the univariate drift condition is satisfied for some  $V : \mathcal{X} \rightarrow [1, \infty]$ ,  $C \subset \mathcal{X}$ ,  $0 < \text{lambda} < 1$ , and  $b < \infty$ . Let  $d = \inf_{x \in C^c} V(x)$ . If  $d > [b/(1 - \text{lambda})] - 1$ , then the bivariate drift condition is satisfied for the same  $C$ , with  $h(x, y) = \frac{1}{2}[V(x) + V(y)]$  and  $\alpha - 1 = \text{lambda} + b/(d + 1) < 1$ .*

**Proof.** (1) Assume  $(x, y) \notin C \times C$ . Then either  $x \notin C$  or  $y \notin C$ , so  $h(x, y) \geq (1 + d)/2$ .

(2) the univariate drift condition applied separately to  $x$  and  $y$  implies that  $PV(x) + PV(y) \leq \text{lambda}V(x) + \text{lambda}V(y) + b$ .

(3) Therefore

$$\begin{aligned} \bar{P}h(x, y) &= \frac{1}{2}[PV(x) + PV(y)] \\ &\leq \frac{1}{2}[\text{lambda}PV(x) + \text{lambda}PV(y) + b] \\ &= \text{lambda}h(x, y) + b/2 \\ &= \text{lambda}h(x, y) + (b/2)[h(x, y)/((1 + d)/2)] \\ &= [\text{lambda} + b/(1 + d)]h(x, y). \end{aligned}$$

which gives the result. □

Now apply these nonuniform quantitative convergence bounds to a Markov chain on an unbounded state space. Let the state space be  $\mathcal{X} = \mathbb{R}$ , the entire real line, with unnormalized target density  $\pi(x) = e^{-|x|}$ . To create a Markov chain which has  $\pi$  as its stationary distribution, we use another version of the Metropolis Algorithm. Each step of the Markov chain proceeds as follows. First, propose to move from the state  $x$  to some other state  $y$ , chosen from the uniform (i.e., Lebesgue) measure on the interval  $[x - 2, x + 2]$ . Then, with probability  $\min\{1, \frac{\pi(x)}{\pi(y)}\}$ , accept this proposal and move to the new state  $y$ , otherwise reject it and remain at  $x$ . Once again, this procedure creates a Markov chain which has  $\pi$  as its stationary distribution. To apply Theorem 21.13, first establish minorization and drift conditions.

**Lemma 21.16.** *The above Markov chain satisfies a minorization condition with  $C = [-2, 2]$ ,  $n_0 = 2$ ,  $\epsilon = \frac{1}{8e^2}$ , and  $\mu(A) = \frac{1}{2} \text{Leb}(A \cap [-1, 1])$ , where  $\text{Leb}$  is Lebesgue measure on  $\mathbb{R}$ .*

**Proof.** (1) Let  $x \in C$ . Without loss of generality, assume  $x \geq 0$ .

(2) First consider  $B \subset [-1, 1]$ , and let  $z \in [0, 1]$  and  $y \in B$ .

(3) Then  $[0, 1] \subset [x - 2, x + 2]$  and  $B \subset [z - 2, z + 2]$ .

(4) Hence the proposal density  $q$  satisfies that  $q(x, z) = q(z, y) = \frac{1}{4}$ .

- (5) Also,  $\pi \leq e^0 = 1$  and  $e^{-1} \leq \pi(y) \leq 1$  and  $\pi(z) \geq e^{-1}$ , so if  $\alpha(x, z) = \min \left[ 1, \frac{\pi(z)}{\pi(x)} \right]$  is the probability of accepting a proposed move from  $x$  to  $z$ , then  $\alpha(x, z) \geq e^{-1}$  and  $\alpha(x, y) \geq e^{-1}$ .

- (6) Hence

$$P^2(x, B) \geq \int_B \int_{x-2}^{x+2} q(x, z) \alpha(x, z) q(z, y) \alpha(z, y) \, dz \, dy \geq \int_B \int_0^1 \frac{1}{4} \cdot \frac{1}{Euler E} \cdot \frac{1}{4} \cdot \frac{1}{Euler E} \, dz \, dy = \frac{1}{16e^2} \text{Leb}(B).$$

- (7) Finally, for any  $A \subset \mathbb{R}$ ,

$$P^2(x, A) \geq P^2(x, A \cap [-1, 1]) \geq \frac{1}{16e^2} \text{Leb}(A \cap [-1, 1]) = \frac{1}{8e^2} \mu(A).$$

□

**Lemma 21.17.** *The above Markov chain satisfies a univariate drift condition with  $V(x) = e^{-|x|/2}$ ,  $C = [-2, 2]$ ,  $\lambda = 0.916$ , and  $b = 0.285$ .*

**Proof.** (1) Without loss of generality, assume  $x \geq 0$ .

- (2) Note

$$PV(x) = \int_{x-2}^{x+2} q(x, y) [V(y) \alpha(x, y) + V(x)(1 - \alpha(x, y))] \, dy.$$

- (3) First compute the integral where  $x \leq y \leq x+2$  where  $\alpha(x, y) = \frac{\pi(y)}{\pi(x)} = \frac{e^{-y}}{e^{-x}} = e^{x-y}$  and  $q(x, y) = \frac{1}{4}$ .

- (4)

$$\begin{aligned} &= \int_x^{x+2} \frac{1}{4} e^{y/2} e^{x-y} \, dy + \int_x^{x+2} \frac{1}{4} e^{x/2} (1 - e^{x-y}) \, dy = \frac{e^x}{4} \int_x^{x+2} e^{-y/2} \, dy + \frac{2e^{x/2}}{4} - \frac{e^{3x/2}}{4} \int_x^{x+2} e^{-y} \, dy \\ &= \frac{e^x}{4} \left[ -2e^{-(x+2)/2} + 2e^{-x/2} \right] + \frac{2e^{x/2}}{4} - \frac{e^{3x/2}}{4} \left[ -e^{-x-2} + e^{-x} \right] \\ &= \frac{e^{x/2}}{4} \left[ -2e^{-1} + 2 + 2 + e^{-2} - 1 \right] \\ &= \frac{1}{4} (3 + e^2 - 2e^{-1}) V(x). \end{aligned}$$

- (5) Let  $\lambda_1 = \frac{1}{4} (3 + e^2 - 2e^{-1}) \approx 0.599894100225$ .

- (6) Note there are three cases:

- (a)  $x \in (2, \infty) \not\subset C = [-2, 2]$ . Then  $\alpha(x, y) = \min[1, \frac{e^{-|y|}}{e^{-|y|}}] = 1$  for all  $y \in (2, \infty)$  so

$$\begin{aligned} PV(x) &= \int_{x-2}^x q(x, y)V(y) \, d(y) + \mathbf{lambda}_1 V(x) \\ &= \frac{1}{4}e^{x/2} \cdot 2 \cdot (1 - e^{-1}) + \mathbf{lambda}_1 V(x) \\ &= \left( \frac{1}{2}(1 - e^{-1}) + \mathbf{lambda}_1 \right) V(x) \leq 0.916V(x) \end{aligned}$$

- (b)  $x \in [1, 2] \subset C = [-2, 2]$ . Again  $\alpha(x, y) = 1$  for all  $y \in [x-2, x]$  so

$$\begin{aligned} PV(x) &= \int_{x-2}^x q(x, y)V(y) \, d(y) + \mathbf{lambda}_1 V(x) \\ &= \frac{1}{4} \left( \int_{x-2}^0 e^{-y/2} \, dy + \int_0^x e^{y/2} \, dy \right) + \mathbf{lambda}_1 V(x) \\ &= \frac{1}{4} \left( \int_0^{2-x} e^{y/2} \, dy + \int_0^x e^{y/2} \, dy \right) + \mathbf{lambda}_1 V(x) \\ &= \frac{1}{2} \left( e^{x/2} + e^{1-x/2} \right) - 1 + \mathbf{lambda}_1 e^{x/2}. \end{aligned}$$

Let  $z = e^{x/2}$ . Computing numerically

$$\max_{x \in [1, 2]} (PV(x) - 0.916V(x)) = \max_{z \in [\sqrt{e}, e]} \left[ \frac{1}{2}(z + e/z) - 1 \right] \mathbf{lambda}_1 z - 0.916z \leq 0.065.$$

(The source gives a value of 0.13, maybe off by a factor of 2 somewhere.)

- (c)  $x \in [0, 1] \subset C$ . Then  $\alpha(x, y) = 1$  for any  $y \in [-x, x]$ .

$$\begin{aligned} PV(x) &= \int_{x-2}^{-x} q(x, y)\alpha(x, y)V(y) + q(x, y)(1 - \alpha(x, y))V(x) \, dy \\ &\quad + \int_{-x}^x q(x, y)V(y) \, dy + \mathbf{lambda}_1 V(x) \\ &= \frac{e^{x/2}}{4} \left[ -2e^{x-1} + e^{2(x-1)} - 2x + 3 \right] + e^{x/2} - 1 + \mathbf{lambda}_1 e^{x/2}. \end{aligned}$$

Computing numerically

$$\max_{x \in [0, 1]} (PV(x) - 0.916V(x)) = 0.285.$$

(Actually, the numerical max is approximately 0.2848331379.)

- (7) Combining the three cases and their symmetric versions for  $x < 0$ ,

$$PV(x) \leq 0.916V(x) + 0.285 \mathbf{1}_C(x).$$

holds for all  $x \in \mathcal{X}$ , as claimed. □

Then apply the Proposition to derive a bivariate drift condition. Note that here  $d = \inf_{x \in C^c} V(x) = e$  and  $[b/(1 - \mathbf{lambda})] - 1 = 2.39 < e$ . So,  $h(x, y) = (V(x) + V(y))$  satisfies a bivariate drift condition with  $\alpha^{-1} = \mathbf{lambda} + b/(d+1) =$

$0.916 + 0.285/(e + 1) \approx 0.99265$ . The quantity  $B_{n_0} = B_2$  also needs a bound. Let  $D = [-6, 6]$ . Then  $P^2(x, D) = 1$  for and  $x \in C$ . Thus

$$\sup_{(x,y) \in C \times C} \bar{R}h(x, y) \leq \sup_{(x,y) \in D \times D} h(x, y) = \sup_{x \in D} V(x) = e^3 < 20.1$$

So

$$B_2 = \max[1, \alpha^2(1 - \epsilon) \sup \bar{R}h] < (0.993)^{-2} \left(1 - \frac{1}{8e^2}\right) (20.1) \approx 20.04$$

Let  $X_0 = 0$ . Then

$$\begin{aligned} \mathbb{E}_{Z \sim \pi} [h(0, Z)] &= \mathbb{E}_{Z \sim \pi} \left[ \frac{1}{2}(V(0) + V(Z)) = \frac{1}{2} + \frac{1}{2} \mathbb{E}_{\pi} [V] \right] \\ &= \frac{1}{2} + \frac{1}{2} \frac{\int_{y \in \mathcal{X}} \text{Euler} E^{\frac{1}{2}|y|} e^{-|y|} dy}{\int_{y \in \mathcal{X}} e^{-|y|} dy} \\ &= \frac{1}{2} + \frac{1}{2} \cdot \frac{2}{1} = 2. \end{aligned}$$

If this specific calculation were not available, then use the bound  $\mathbb{E}_{\pi} [V] \leq b/(1 - \text{lambda}) = 0.285/(1 - 0.916) = 3.393$  as discussed above. Therefore, by Theorem 2, with  $X_0 = 0$ ,

$$\| \text{dist}(X_n) - \pi(\cdot) \|_{TV} \leq (1 - \epsilon)^j + \alpha^{-n} B_2^{j-1} \mathbb{E}_{Z \sim \pi y} [h(0, Z)] \leq (0.983)^j + [(0.993)^n (20.04)^{j-1}].$$

The chain is within 0.01 of stationarity after 120,000 iterations. This is quite a conservative upper bound. Nevertheless, this is a concrete quantitative convergence bound for an unbounded Markov chain.

### 21.7. Chapter Ending Answer

Since  $P$  is irreducible and aperiodic, there exist  $r$  such that  $P^r$  has strictly positive entries. Let  $\Pi$  be the matrix with  $\text{card}(\mathcal{X}) = k$  rows, each of which is the row vector  $\pi$ . For sufficiently small  $\delta > 0$ ,  $(P^r)_{ij} \geq \delta \pi_j$  for  $i, j \in \mathcal{X}$ .

In this chapter, this estimate is relaxed to the minorization condition.

### 21.8. Chapter Summary

#### Key Concepts.

- (1)
- (2)
- (3)

#### Vocabulary.

- (1) A Markov chain with state space  $\mathcal{X}$  and transition probabilities  $P$  satisfies a **minorization condition** if there exists a (measurable) subset  $C \subset \mathcal{X}$ , a probability measure  $\nu$  on  $\mathcal{X}$ , a constant  $\epsilon > 0$ , and a positive integer  $n_0$ , such that

$$P^{n_0}(x, \cdot) \geq \epsilon \nu(\cdot), x \in C.$$

- (2) Such a set  $C$  satisfying the minorization condition is a **small set**.

- (3) In particular, if  $C = X$  (the entire state space), then the Markov chain satisfies a **uniform minorization condition**, also referred to as *Doebelin's condition*.
- (4) Replacing the distribution  $\nu(\cdot)$  with  $\nu_{xy}(\cdot)$ , allowing it to depend on  $x$  and  $y$ , then  $C$  is called a **pseudo-small set**.
- (5) A Markov chain with a small set  $C \subset \mathcal{X}$  satisfies a **bivariate drift condition** if there exists a function

$$h : \mathcal{X} \times \mathcal{X} \rightarrow [1, \infty)$$

and some  $\alpha > 1$  such that

$$\bar{P}h(x, y) \leq h(x, y)/\alpha$$

where

$$\bar{P}h(x, y) := \mathbb{E}[h(X_{n+1}, Y_{n+1}) \mid X_n = x, Y_n = y]$$

is the expected or average value of  $h(x_{n+1}, y_{n+1})$  on the next iteration, when the chains start from  $x$  and  $y$  respectively and proceed independently.

- (6) A Markov chain with a small set  $C$  satisfies a **univariate drift condition** if there are constants  $0 < \text{lambda} < 1$  and  $b < \infty$ , and a function  $V : \mathcal{X} \rightarrow [1, \infty]$ , such that

$$PV(x) \leq \text{lambda}V(x) + b\mathbf{1}_C(x), \quad x \in \mathcal{X}$$

where  $PV(x) = \mathbb{E}[V(X_n + 1) \mid X_n = x]$ .

#### Notation.

- (1)  $X$  and  $Y$  be 2 random variables.  $A$  is any subset of  $\mathbb{R}$ .
- (2)  $\mathcal{L}(X)$  is the probability law for  $X$ .
- (3) Total variation distance between  $X$  and  $Y$  is  $\|\mathcal{L}(X) - \mathcal{L}(Y)\|_{TV}$ .
- (4) A Markov chain with state space  $\mathcal{X}$  and transition probabilities  $P$ .
- (5) A measurable subset  $C \subset \mathcal{X}$ .
- (6) A probability measure  $\nu$  on  $\mathcal{X}$ .
- (7) A constant  $\epsilon > 0$ .
- (8) A positive integer  $n_0$ .

### 21.9. Sources

This section is adapted from:

#### 21.10. Reading Suggestion:

#### 21.11. Outside Readings and Links:

- (1)
- (2)
- (3)
- (4)



Chapter 1: Markov Chains.

- 1.1: (a) There are 4 states,  $D$  for dropping out, 1 for first-year, 2 for second-year, and  $G$  for graduating.

$$P = \begin{array}{c} \begin{array}{cccc} & D & 1 & 2 & G \\ D & \left( \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 3/20 & 1/4 & 3/5 & 0 \\ 1/10 & 0 & 1/5 & 7/10 \\ 0 & 0 & 0 & 1 \end{array} \right) \\ 1 \\ 2 \\ G \end{array} \end{array}.$$

- (b) Absorbing states are  $D$  and  $G$ . Transient states are 1, 2.

(c)

$$P^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 99/400 & 1/16 & 27/100 & 21/50 \\ 3/25 & 0 & 1/25 & 21/25 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Probability of graduating on time is  $21/50$ .

$$P^3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2271/8000 & 1/64 & 183/2000 & 609/1000 \\ 31/250 & 0 & 1/125 & 217/250 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

- (d) Probability of graduating in 3 years is  $609/1000$ .

(e) Canonical form is

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 3/20 & 0 & 1/4 & 3/5 \\ 1/10 & 7/10 & 0 & 1/5 \end{pmatrix}$$

so

$$N = \begin{pmatrix} 4/3 & 1 \\ 0 & 5/4 \end{pmatrix} \quad B = NA = \begin{pmatrix} 3/10 & 7/10 \\ 1/8 & 7/8 \end{pmatrix}.$$

The chance that a student will graduate eventually is  $7/10$ . The chance the student will drop out eventually is  $3/10$ .

- (f) The expected time to graduation is  $4/3 + 1 = 7/3$  years.

Problem created by LT Grant, 2006.

- 1.2: (a)

$$P = \begin{array}{c} \begin{array}{cccccc} & A & B & C & D & E & F \\ A & \left( \begin{array}{cccccc} 0 & 1/3 & 1/3 & 0 & 1/3 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 1/3 & 1/3 & 0 & 0 & 1/3 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right) \\ B \\ C \\ D \\ E \\ F \end{array} \end{array}.$$

- (b) Absorbing states are  $E$  and  $F$ . Transient states are  $A, B, C, D$ .

(c)

$$P' = \begin{matrix} & E & F & A & B & C & D \\ \begin{matrix} E \\ F \\ A \\ B \\ C \\ D \end{matrix} & \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 1/3 & 1/3 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 \\ 0 & 1/3 & 0 & 1/3 & 1/3 & 0 \end{pmatrix} \end{matrix}.$$

$$N = \begin{pmatrix} 2 & 1 & 1 & 1 \\ \frac{3}{2} & 2 & 1 & \frac{3}{2} \\ \frac{3}{2} & 1 & 2 & \frac{3}{2} \\ 1 & 1 & 1 & 2 \end{pmatrix}.$$

(d)  $(N\mathbf{1})_1 = 2 + 1 + 1 + 1 = 5$ .(e) From  $A$ , probability to  $E$  is  $2/3$ , to  $F$  is  $1/3$ . From  $D$ , probability to  $E$  is  $1/3$ , to  $F$  is  $2/3$ . Seems reasonable by symmetry.

Problem created by LT Grant, 2006.

1.3: (a) Expect absorption probabilities from  $B$  to  $E$  to increase and absorption probability of  $B$  to  $F$  to decrease.(b) From  $A$ , probability to  $E$  to increase, to  $F$  to decrease. From  $D$ , probability to  $E$  to increase, to  $F$  to decrease.

(c)

$$\begin{pmatrix} 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

(d) From  $A$ , probability to  $E$  increases to  $0.792$ , to  $F$  decreases to  $0.208$ . From  $D$ , probability to  $E$  increases to approximately  $0.458$ , to  $F$  decreases to approximately  $0.542$ .

Problem created by LT Grant, 2006.

1.4:

$$P_{ij} = \begin{cases} (\frac{i}{N})^2 & j = i - 1, & i = 1, 2, \dots, N \\ (2\frac{i}{N})\frac{N-i}{N} & j = i, & i = 0, 1, 2, \dots, N \\ 1 - (\frac{i}{N})^2 & j = i + 1, & i = 0, 1, 2, \dots, N - 1 \\ 0 & \text{otherwise} \end{cases}$$

There are no absorbing states.

As an example, for  $N = 3$ , the transition probability matrix is

$$\begin{matrix} & 0 & 1 & 2 & 3 \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/9 & 4/9 & 4/9 & 0 \\ 0 & 4/9 & 4/9 & 1/9 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{matrix}$$

with stationary distribution  $\pi = (1/20, 9/20, 9/20, 1/20)$  For  $N = 4$ , the transition probability matrix is

$$\begin{matrix} & 0 & 1 & 2 & 3 & 4 \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1/16 & 6/16 & 9/16 & 0 & 0 \\ 0 & 4/16 & 8/16 & 4/16 & 0 \\ 0 & 0 & 9/26 & 6/16 & 1/16 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \end{matrix}$$

Adapted from Karlin and Taylor, *A First Course in Stochastic Processes*, second edition, page 73, problem 1(b).

1.5:

$$P_{ij} = \begin{cases} \left(\frac{i}{N}\right)q & j = i - 1, & i = 1, 2, \dots, N \\ \left(\frac{i}{N}\right)p + \left(\frac{N-i}{N}\right)q & j = i, & i = 0, 1, 2, \dots, N \\ \left(1 - \frac{i}{N}\right)p & j = i + 1, & i = 0, 1, 2, \dots, N - 1 \\ 0 & \text{otherwise} \end{cases}$$

An example in the case  $N = 4$

$$\begin{pmatrix} q & p & 0 & 0 & 0 \\ \frac{q}{4} & \frac{3q}{4} + \frac{p}{4} & \frac{3p}{4} & 0 & 0 \\ 0 & \frac{q}{2} & \frac{q}{2} + \frac{p}{2} & \frac{p}{2} & 0 \\ 0 & 0 & \frac{3q}{4} & \frac{q}{4} + \frac{3p}{4} & \frac{p}{4} \\ 0 & 0 & 0 & q & p \end{pmatrix}.$$

The unnormalized stationary distribution is  $[1, 4p/q, 6p^2/q^2, 4p^3/q^3, p^4/q^4]$ , for  $p = 1/2 = q$ , normalized, this is  $[1/16, 1/4, 3/8, 1/4, 1/16]$ , for  $p = 3/4, q = 1/4$ , normalized, this is approximately  $[0.004, 0.047, 0.211, 0.422, 0.316]$ .

There are no absorbing or transient states.

Adapted from Karlin and Taylor, *A First Course in Stochastic Processes*, second edition, page 74, problem 2(a).

1.6:

$$P_{ij} = \begin{cases} \left(1 - \frac{i}{N}\right)p & j = i - 1, & i = 1, 2, \dots, N \\ \left(\frac{i}{N}\right)p + \left(\frac{N-i}{N}\right)q & j = i, & i = 0, 1, 2, \dots, N \\ \left(\frac{i}{N}\right)q & j = i + 1, & i = 0, 1, 2, \dots, N - 1 \\ 0 & \text{otherwise} \end{cases}$$

There are no absorbing or transient states.

Adapted from Karlin and Taylor, *A First Course in Stochastic Processes*, second edition, page 74, problem 2(b).

1.7: From numerical experiments with the transition probability matrix, slightly more than 50% of the time. This matrix converges fairly slowly to the limiting matrix, so experiments require about  $P^{50}$ .

Adapted from FiveThirtyEight Riddler who in turn got the problem from Steve Simon.

1.8: Keep track of the different “states” of Louie’s umbrellas at home at the end of the work day. He could have 3 at home and 0 at work, 2 at home and 1 at

work and so on. In this solution, there are five states: 0, 1, 2 or 3 umbrellas at home plus the state in which Louie has already gotten wet. The rows of the matrix are Louie's current state, and the columns are his destination. For example, he starts in the third row (2 umbrellas at home and 1 at work). There is no chance he will end the day with zero umbrellas at home since he always has an umbrella available, there is a  $0.3 = 0.5 \cdot 0.6$  chance he will end the day with just 1 at home (from rain in the morning and no rain in the afternoon), a 0.5 chance with 2 at home, a 0.2 chance with 3 at home, and no chance he will get wet on this first day since he always has an umbrella available.

The movement through the random states of a day is described by the transition matrix, which contains the probabilities of umbrellas moving from 1 place to another on any given day. The transition probability matrix is:

$$\begin{pmatrix} 0.3 & 0.2 & 0.0 & 0.0 & 0.5 \\ 0.3 & 0.5 & 0.2 & 0.0 & 0.0 \\ 0.0 & 0.3 & 0.5 & 0.2 & 0.0 \\ 0.0 & 0.0 & 0.3 & 0.5 & 0.2 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{pmatrix}.$$

To get the probabilities for the entire work week, simply multiply this matrix by itself five times, representing the umbrella transitions due to meteorological randomness over the five days, which gives

$$\begin{pmatrix} 0.04791 & 0.07634 & 0.04976 & 0.01776 & 0.80823 \\ 0.11451 & 0.19889 & 0.15274 & 0.06752 & 0.46634 \\ 0.11196 & 0.22911 & 0.22553 & 0.12610 & 0.3073 \\ 0.05994 & 0.15192 & 0.18915 & 0.12425 & 0.47474 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Last, look at the third row (the state in which he began) and the final column: That's the chance he gets wet during the week. Subtract from 1 to find the chance that he didn't get wet and get 69.27 percent.

Adapted from FiveThirtyEight Riddler who in turn got the problem from Josh Vandenharm.) This problem and the solution as a Markov chain appeared in FiveThirtyEight Riddler column of December 14, 2018.

This is a version of Ross, page 181, problem number 22.

- 1.9: A random walk on the 2-dimensional integer lattice, started off the  $x$ -axis, with the rule that on reaching the  $x$ -axis the chain continues on the  $x$ -axis as a 1-dimensional random walk has an infinite absorbing set, namely the  $x$ -axis. If instead, upon reaching the  $x$ -axis, the chain remains at the hitting point, then the chain has infinitely many absorbing states. This problem is adapted from W. Feller, *An Introduction to Probability Theory and Its Applications*, 3rd Edition, 1957, Jon Wiley and Sons Example XV.4.d, page 386.

Chapter 2: Classes of States and Stationary Distributions.

- 2.1: (a)

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(b)

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ or } \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

(c)

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(d)

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

State 2 communicates with states 1 and 3, but that is all.

(e)

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

2.2: The 4 states are the number of balls in urn  $A$ , from 0 to 3.

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

In this Markov chain all states communicate, are positive recurrent, are aperiodic, and there are no absorbing or transient states, the Markov chain is irreducible. The stationary distribution is  $\pi = [1/4, 1/4, 1/4, 1/4]$  so in the long run urn  $A$  spends 1/4 of the time empty. This does not depend on the initial distribution of balls.

2.3: Label the  $2(n+1)$  states as  $(H, k, n-k)$  or  $(W, k, n-k)$  indicating (redundantly) as starting the trip from Home with  $k$  umbrellas at home, and  $n-k$  umbrellas at Work. Enumerate the states of the Markov chain successively as

1::  $(H, 0, n)$  is the state of starting from home with 0 umbrellas at home and  $n$  at work.

2::  $(W, 0, n)$  is the state of starting from work with 0 umbrellas at home and  $n$  at work.

: ...

$2n-1$ ::  $(H, n-1, 1)$  the state of starting from home with  $n-1$  umbrellas and 1 at work.

$2n$ ::  $(W, n-1, 1)$  is the state of starting from work with  $n-1$  umbrellas at home and 1 at work.

$2n+1$ ::  $(H, n, 0)$  is the state of starting from home with  $n$  umbrellas at home and 0 at work.

$2n+2$ ::  $(W, n, 0)$  is the state of starting from work with  $n$  umbrellas at home and 0 at work.

Then the transition probability matrix is

$$\begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & \dots & 0 & 0 & 0 \\ \dots & & & & & & \\ 0 & 0 & 0 & \dots & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$

It is easiest to examine a small case, say  $n = 3$  and extrapolate from that concrete example. For  $n = 3$ , the probability transition matrix is

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

Then solving  $\pi = \pi P$  for this small case ( $n = 3$ ) suggests that the solution is  $\pi = (1/(2(2n+1)), 1/(2n+1), \dots, 1/(2n+1), 1/(2(2n+1)))$ . Then it is easy to verify that indeed this is a stationary probability distribution. The professor gets wet when he starts from home with all the umbrellas at work, or starts from work with all the umbrellas at home, (the first and last states) and it is raining. The probability of this, in the long run or asymptotically is

$$\frac{1}{2} \cdot \frac{1}{2(2n+1)} + \frac{1}{2} \cdot \frac{1}{2(2n+1)} = \frac{1}{2(2n+1)}.$$

All states are accessible from each other and therefore the Markov chain is irreducible. It is easy to multiply the transition probability matrix against itself, and see that  $P_{ii}^2 = 1/2$  except for  $i = 2$  and  $i = 2n + 1$  where the value is  $3/4$ . Therefore, each state is periodic of period 2.

2.4: The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & 1/2 \\ 0 & 1/2 & 0 & 0 & 1/4 & 1/4 \\ 0 & 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ r/2 & q/2 & p/2 & 0 & 1/2 & 0 \\ r/2 & q/2 & 0 & p/2 & 0 & 1/2 \end{pmatrix} \end{matrix}.$$

The stationary distribution is

$$\left( \frac{r}{2}, \frac{q}{2}, \frac{p(q+2p)}{4}, \frac{p(2r+q)}{4}, \frac{q+2p}{4}, \frac{2r+q}{4} \right).$$

2.5: See the next solution with  $v = 1/3$ .

2.6: Using the assumption that the bathroom is occupied  $1 - v$  of the time, and vacant  $v$  of the time, all day, every day, the transition from state to state each minute is a Markov chain with transition probability

$$\begin{array}{cc} & \begin{array}{cc} O & V \end{array} \\ \begin{array}{c} O \\ V \end{array} & \begin{pmatrix} 1-v & v \\ 1-v & v \end{pmatrix} \end{array}.$$

It is easy to see that this chain is irreducible, positive recurrent and aperiodic. The stationary distribution is  $(1 - v, v)$ , consistent with the assumption that the bathroom is occupied  $1 - v$  of the time, all day, every day.

The possible transitions at each minute are:

- (1) A Conscientious person is in the bathroom, and it is Occupied and the sign says Occupied. This state is  $OCO$ . Either the person stays and the state remains Occupied with sign Occupied with probability  $1 - v$ , or the conscientious person leaves and the state is  $VV$  with probability  $r \cdot v$ .
- (2) A Forgetful person is in the bathroom, and it is Occupied and the sign says Occupied. This state is  $OFO$ . Either the person stays and the state remains Occupied with sign Occupied with probability  $1 - v$ , or the forgetful person leaves and the state is  $VO$  with probability  $(1/2) \cdot v = v/2$  or the forgetful person leaves, changing the sign and the state is  $VV$  with probability  $1/2 \cdot v = v/2$ .
- (3) An Oblivious person is in the bathroom, and it is Occupied and the sign says Occupied. Name this state as  $OOO$ . Either the person stays and the state remains Occupied with sign Occupied with probability  $1 - v$ , or the oblivious person leaves and the state is  $VO$  with probability  $v$ .
- (4) A Oblivious person is in the bathroom, and it is Occupied but the sign says Vacant. Name this state as  $OOV$ . Either the person stays and the state remains Occupied with sign Vacant with probability  $1 - v$ , or the oblivious person leaves and the state is  $VV$  with probability  $v$ .
- (5) The bathroom is Vacant, but the sign says Occupied. With probability  $1 - v$  some person will approach, nevertheless try the door and find the true state of vacancy and enter, dealing with the sign according to their type. Then the transition is to  $OCO$  with probability  $r(1 - v)$ ,  $OFO$  with probability  $q(1 - v)$  and  $OOO$  with probability  $p(1 - v)$ . With probability  $v$  the state remains  $VO$ .
- (6) The bathroom is Vacant, and the sign says Vacant. With probability  $1 - v$  some person will approach, nevertheless try the door and easily find the true state of vacancy and enter, dealing with the sign according to their type. Then the transition is to  $OCO$  with probability  $r(1 - v)$ ,  $OFO$  with probability  $q(1 - v)$  and  $OOV$  with probability  $p(1 - v)$ . With probability  $v$  the state remains  $VV$ .

The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1-v & 0 & 0 & 0 & 0 & v \\ 0 & 1-v & 0 & 0 & v/2 & v/2 \\ 0 & 0 & 1-v & 0 & v & 0 \\ 0 & 0 & 0 & 1-v & v & 0 \\ r(1-v) & q(1-v) & p(1-v) & 0 & v & 0 \\ r(1-v) & q(1-v) & 0 & p(1-v) & 0 & v \end{pmatrix} \end{matrix}.$$

The stationary distribution is:

$$\left( r(1-v), q(1-v), \frac{p(q+2p)(1-v)}{2}, \frac{p(2r+q)(1-v)}{2}, \frac{(q+2p)v}{2}, \frac{(2r+q)v}{2} \right).$$

As  $v \rightarrow 1$ , the stationary distribution tends to  $(0, 0, 0, 0, \frac{(q+2p)}{2}, \frac{(2r+q)}{2})$ . As  $v \rightarrow 0$ , the stationary distribution tends to  $(r, q, \frac{p(q+2p)}{2}, \frac{p(2r+q)}{2}, 0, 0)$ .

2.7: Suppose the probability of an oblivious person entering the bathroom is  $w$ . Then proportion of time that the bathroom is occupied by an oblivious person is  $p(1-w)$ . Likewise, and as in the previous problem, the proportion of time the bathroom is occupied by forgetful and conscientious people is  $q(1-v)$  and  $r(1-v)$  respectively. If the probabilities of occupancy by forgetful and conscientious people are both equal to  $1-v$  then the assumption that oblivious people spend twice as much time in the bathroom is  $p(1-w) = 2(q+r)(1-v)$  or  $w = 1 - \frac{2(q+r)}{p}(1-v) = 1 - \frac{2(1-p)}{p}(1-v)$ . Since  $0 < w < 1$ , this puts some restrictions depending on  $p$  and  $v$ .

The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1-v & 0 & 0 & 0 & 0 & v \\ 0 & 1-v & 0 & 0 & v/2 & v/2 \\ 0 & 0 & 1-w & 0 & w & 0 \\ 0 & 0 & 0 & 1-w & w & 0 \\ r(1-v) & q(1-v) & p(1-v) & 0 & v & 0 \\ r(1-v) & q(1-v) & 0 & p(1-v) & 0 & v \end{pmatrix} \end{matrix}.$$

2.8: (1) First consider the statement: If  $i$  and  $j$  communicate, and  $i$  is recurrent, then so is  $j$ .

- (a) If  $i$  and  $j$  communicate, then there is an  $r > 0$  such that  $(P^r)_{ji} > 0$  and an  $s > 0$  such that  $(P^s)_{ij} > 0$ .
- (b) If  $i$  is recurrent, then  $\sum_{n=1}^{\infty} (P^n)_{ii} = \infty$  so also  $\sum_{n=r+s+1}^{\infty} (P^n)_{ii} = \infty$ .
- (c)  $(P^n)_{jj} > (P^r)_{ji}(P^{n-r-s})_{ii}(P^s)_{ij}$ , that is the probability of going from  $j$  to  $j$  is greater than the probability of an excursion from  $j$  to  $i$ , then from  $i$  to  $i$ , and from  $i$  to  $j$ .



(d) Then

$$\begin{aligned} \sum_{n=1}^{\infty} (P^n)_{jj} &> \sum_{n=r+s+1}^{\infty} (P^r)_{ji} (P^{n-r-s})_{ii} (P^s)_{ij} = \\ &= (P^r)_{ji} \left( \sum_{n=r+s+1}^{\infty} (P^{n-r-s})_{ii} \right) (P^s)_{ij} = \infty \end{aligned}$$

Therefore,  $j$  is recurrent.

- (2) Suppose  $i$  and  $j$  communicate, and  $i$  is transient, but  $j$  is recurrent. Since  $j$  communicates with  $i$  and  $j$  is recurrent, by the previous proof then  $i$  must be recurrent, a contradiction. Therefore,  $j$  must be transient.
- (3) The statement follows from the definition of irreducible and the previous proofs.

2.9: The recursive equation can be interpreted by considering paths for which  $X_0 = i$  and  $X_n = j$  and the first return to state  $j$  occurs at step  $k$ . The probability that the first return is at step  $k$  is  $f_{ij}^k$  and the probability of then going from state  $j$  to state  $j$  in  $n-k$  steps, independent of the past, is  $(P^{n-k})_{jj}$ . Adding over all the disjoint possible first arrivals from  $i$  to  $j$  gives the recursive equation.

2.10: Let  $\epsilon > 0$  be given. Choose  $N_1$  so large that  $|a_n - a| < \epsilon/2$  for  $n > N_1$ . Choose  $N_2 > N_1$  so large that  $\frac{1}{n} \sum_{\nu=1}^{N_1} |a_\nu - a| < \epsilon/2$  for  $n > N_2$ . Then for  $n > N_2$ ,

$$\begin{aligned} \left| \frac{1}{n} \sum_{\nu=1}^n a_\nu - a \right| &\leq \frac{1}{n} \sum_{\nu=1}^{N_1} |a_\nu - a| + \frac{1}{n} \sum_{\nu=N_1+1}^n |a_\nu - a| \\ &\leq \frac{1}{n} \sum_{\nu=1}^{N_1} |a_\nu - a| + \frac{1}{n} \sum_{\nu=N_1+1}^n |a_\nu - a| \\ &< \frac{\epsilon}{2} + \frac{1}{n} \sum_{\nu=N_1+1}^n \frac{\epsilon}{2} \\ &< \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon. \end{aligned}$$

Therefore

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n a_\nu = a,$$

2.11: By induction it is enough to prove  $\lim_{j \rightarrow \infty} u_{n_j-1} = \mu$ .

From the hypotheses on  $a_k$  and  $b_k$ , it follows by induction that  $u_n \geq 0$  for all  $n$ . Recall that  $\mu = \liminf_{n \rightarrow \infty} u_n$  with a subsequence such that  $\lim_{j \rightarrow \infty} u_{n_j} = \mu$ . For purposes of proof by contradiction, suppose that  $\lim_{j \rightarrow \infty} u_{n_j-1} \neq \mu$ . Then there exists a value  $\mu' > \mu$  such that  $u_{n_j-1} > \mu'$  for an infinite number of  $j$ . Let  $\epsilon = \min \{1, a_1(\mu' - \mu)/L\} > 0$  where  $L > \mu + a_1 + 3$ . For the given  $\epsilon$  determine  $N(\epsilon)$  so large that

$$\sum_{k=0}^{N(\epsilon)} a_k > 1 - \epsilon$$

or equivalently

$$\sum_{k=N(\epsilon)+1}^{\infty} a_k < \epsilon$$

Now let  $j$  be chosen so large that  $n_j > N(\epsilon)$  and  $u_{n_j} < \mu + \epsilon$  (possible since  $\lim_{j \rightarrow \infty} u_{n_j} = \mu$ ) and add additionally  $j$  so large that  $u_{n_j-1} > \mu'$  (possible since  $u_{n_j-1} > \mu'$  for an infinite number of  $j$ ) and finally  $u_n > \mu - \epsilon$  for  $n > n_j - N(\epsilon)$  (possible since  $\mu = \liminf_{n \rightarrow \infty} u_n$ ). This set of choices using  $\epsilon$  and  $N(\epsilon)$  establishes a large value of  $j$  with corresponding large  $n_j$ .

Since  $b_n \geq 0$ , the renewal equation implies

$$\begin{aligned} u_{n_j} &\geq \sum_{k=0}^{n_j} a_k u_{n_j-k} \\ &= \sum_{k=0}^{N(\epsilon)} a_k u_{n_j-k} + \sum_{k=N(\epsilon)+1}^{n_j} a_k u_{n_j-k} \\ &\geq \sum_{k=0}^{N(\epsilon)} a_k u_{n_j-k} \\ &= (a_0 u_{n_j} + a_2 u_{n_j-2} + \cdots + a_{N(\epsilon)} u_{n_j-N(\epsilon)}) + a_1 u_{n_j-1} \\ &\geq (a_0 + a_2 + \cdots + a_{N(\epsilon)})(\mu - \epsilon) + a_1 \mu' \\ &> (1 - \frac{\epsilon}{M} - a_1)(\mu - \epsilon) + a_1 \mu' \\ &= \mu - \epsilon \mu - a_1 \mu - \epsilon(1 - \epsilon - a_1) + a_1 \mu' \\ &= \mu + a_1(\mu' - \mu) - \epsilon \mu - \epsilon(1 - \epsilon - a_1) \\ &= \mu + L\epsilon - \epsilon(\mu + 1 - \epsilon - a_1) \\ &= \mu + \epsilon(L - 1 - \epsilon - \mu + a_1) \\ &> \mu + \epsilon(L - 1 - 1 - \mu + a_1). \end{aligned}$$

By the choice of  $L$  the last expression is greater than  $\mu + \epsilon$ , a contradiction, establishing the result.

2.12: It is immediate that  $\pi_1 = \frac{1}{p}\pi_0$ . By induction  $\pi_i = \frac{(1-p)^{i-1}}{p^i}\pi_0$ . The normalization condition is

$$\pi_0 \left( 1 + \frac{1}{p} + \frac{(1-p)}{p^2} + \frac{(1-p)^2}{p^3} + \cdots \right) = 1.$$

Now is apparent why  $p > 1/2$  is necessary for stationarity. The normalization simplifies to  $\pi_0 \left( 1 + \frac{1}{2p-1} \right) = 1$ . Then  $\pi_\nu = \frac{2p-1}{2p} \left( \frac{(1-p)^{\nu-1}}{p^\nu} \right)$  for  $\nu \geq 1$ .

Chapter 3: Waiting Time to Absorption.

3.1: This leads to the single-step transition matrix  $P$  partitioned into one absorbing state for “leave firm” and three transient states: junior lawyer, senior

lawyer, partner

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.05 & 0.80 & 0.15 & 0 \\ 0.10 & 0 & 0.70 & 0.20 \\ 0.05 & 0 & 0 & 0.95 \end{pmatrix}.$$

The transient transition matrix is

$$T = \begin{pmatrix} 0.80 & 0.15 & 0 \\ 0 & 0.70 & 0.20 \\ 0 & 0 & 0.95 \end{pmatrix}.$$

The corresponding fundamental matrix is

$$N = (I_3 - T)^{-1} = \begin{pmatrix} 5 & 5/2 & 10 \\ 0 & 10/3 & 40/3 \\ 0 & 0 & 20 \end{pmatrix}.$$

The waiting times to absorption are then

$$(I - T)^{-1}\mathbf{1} = (35/2, 50/3, 20)^T.$$

Now compute the covariances for the first transient state, junior lawyer. Using

$$\text{diag } N_{(1,\cdot)}N + N^T \text{diag } N_{(1,\cdot)} - N_{(1,\cdot)}^T N_{(1,\cdot)} - \text{diag } N_{(1,\cdot)}$$

gives

$$\text{Cov}[Y_{1j}, Y_{1k}] = \begin{pmatrix} 20 & 0 & 0 \\ 0 & 95/12 & 25/3 \\ 0 & 25/3 & 290 \end{pmatrix} = \begin{pmatrix} 20 & 0 & 0 \\ 0 & 7.91667 & 8.33333 \\ 0 & 8.33333 & 290 \end{pmatrix}.$$

Since  $w_i = \sum_{j=a+1}^t Y_{ij}$ , using  $\text{Var}[w_i] = \sum_{j=a+1}^t \sum_{l=a+1}^t \text{Cov}[Y_{1j}, Y_{1l}]$ , the variance is the sum of the entries in the covariance matrix. Hence  $\text{Var}[w_1] = 334.58$  (in units of year<sup>2</sup>). The standard deviation is 18.29 years. As a point of special interest, note that the standard deviation is larger than the mean so that knowing the mean is not enough to understand how long a junior lawyer will be with the firm.

3.2: Theorem 3.3 gives the variances of the waiting times as

$$\text{Var}[\mathbf{w}] = (2N - I)N\mathbf{1} - (N\mathbf{1})_{\text{sq}}.$$

Using the matrix  $N$  from the test example, this is

$$\begin{pmatrix} \frac{551592}{476496} \\ \frac{7225}{83352} \\ \frac{1445}{15264} \\ \frac{289}{330312} \\ \frac{7225}{247536} \\ \frac{7225}{5400} \\ \frac{289}{289} \end{pmatrix}$$

or approximately

$$\begin{pmatrix} 76.345 \\ 65.951 \\ 57.683 \\ 52.817 \\ 45.718 \\ 34.261 \\ 18.685 \end{pmatrix}$$

The entry for 0 rounds to 52.81661, the same as the variance in the text example.

3.3: For  $1 \leq j \leq 5$ , let  $p_j$  be the probability that the frog eventually reaches pad 10 starting at pad  $j$ . By symmetry  $p_5 = \frac{1}{2}$ . For the frog to reach pad 10 starting from pad 4, the frog goes either to pad 3 with probability  $\frac{2}{5}$  or to pad 5 with probability  $\frac{3}{5}$ , and then continues on a successful sequence from either of these pads. Thus  $p_4 = \frac{2}{5}p_3 + \frac{3}{5}p_5 = \frac{2}{5}p_3 + \frac{3}{10}$ . Similarly, to reach pad 10 starting from pad 3, the frog goes either to pad 2 with probability  $\frac{3}{10}$  or to pad 4 with probability  $\frac{7}{10}$ . Thus  $p_3 = \frac{3}{10}p_2 + \frac{7}{10}p_4$ , and substituting from the previous equation for  $p_4$  gives  $p_3 = \frac{5}{12}p_2 + \frac{7}{24}$ . In the same way,  $p_2 = \frac{1}{5}p_1 + \frac{4}{5}p_3$  and after substituting for  $p_3$  gives  $p_2 = \frac{3}{10}p_1 + \frac{7}{20}$ . Lastly, for the frog to escape starting from pad 1, it is necessary for it to get to pad 2 with probability  $\frac{9}{10}$ , and then escape starting from pad 2. Thus  $p_1 = \frac{9}{10}p_2 = \frac{9}{10}(\frac{3}{10}p_1 + \frac{7}{20})$ , and solving the equation gives  $p_1 = \frac{63}{146}$ .

This problem and solution are from the 2014 AMC 12 B, number 22.

3.4: Use first-step analysis, setting up a system of linear equations in which each variable represents the probability that the goal (in this case, that the frog ends at a vertical side of the square) is achieved from a specific location. In this case there are 9 internal locations, so the system will have 9 variables and 9 equations. Exploiting the symmetry of this problem can reduce the number of variables and equations to 4. Let  $m$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(2, 2)$ ; let  $c$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(1, 3)$ ,  $(3, 3)$ ,  $(3, 1)$ , or  $(1, 1)$ ; let  $v$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(1, 2)$  or  $(3, 2)$ ; and let  $h$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(2, 1)$  or  $(2, 3)$ . (These letters were chosen to stand for middle, center, vertical, and horizontal, respectively.) Because the probability of a move left, right, down, or up at each step is  $\frac{1}{4}$ , these variables must satisfy the following system:

$$\begin{aligned} m &= \frac{1}{2}v + \frac{1}{2}h \\ c &= \frac{1}{4} + \frac{1}{4}v + \frac{1}{4}h \\ v &= \frac{1}{4} + \frac{1}{4}m + \frac{1}{2}c \\ h &= \frac{1}{2}m + \frac{1}{2}c. \end{aligned}$$

The solution of this system is  $m = \frac{1}{2}$  (which in retrospect is obvious by symmetry),  $c = \frac{1}{2}$  (also obvious by symmetry),  $v = \frac{5}{8}$  (the requested probability), and  $h = \frac{3}{8}$ .

This problem and solution are from the 2020 AMC 12A, number 11.

3.5: The game neither adds nor subtracts the number of balls in use at any turn of the game, so  $a + b + c = n$  is fixed. Then it is sufficient to keep track of the number of balls in urns A and B in any turn. Let  $D_{a,b} = \mathbb{E}[\tau | N_{a,b}]$  be the expected duration of the game when the urn A has  $a$  balls, urn B has  $b$  balls, and urn C has  $c = n - a - b$  balls. Using first-step analysis:

- urn A has  $a + 1$  balls, urn B has  $b - 1$  balls and urn C has  $n - a - b$  balls with probability  $1/6$ ,
- urn A has  $a + 1$  balls, urn B has  $b$  balls and urn C has  $n - a - b - 1$  balls with probability  $1/6$ ,
- urn A has  $a - 1$  balls, urn B has  $b + 1$  balls and urn C has  $n - a - b$  balls with probability  $1/6$ ,
- urn A has  $a$  balls, urn B has  $b + 1$  balls and urn C has  $n - a - b - 1$  balls with probability  $1/6$ ,
- urn A has  $a - 1$  balls, urn B has  $b$  balls and urn C has  $n - a - b + 1$  balls with probability  $1/6$ ,
- urn A has  $a$  balls, urn B has  $b - 1$  balls and urn C has  $n - a - b + 1$  balls with probability  $1/6$ .

Then

$$D_{a,b} = (1/6)[D_{a+1,b-1} + D_{a+1,b} + D_{a-1,b+1} + D_{a,b+1} + D_{a-1,b} + D_{a,b-1}] + 1$$

The boundary conditions are

- (1)  $D_{0,b} = 0$  for  $0 \leq b \leq n$ ,
- (2)  $D_{a,0} = 0$  for  $0 \leq a \leq n$ ,
- (3)  $D_{a,b} = 0$  for  $a + b = n$ .

The solution of this non-homogeneous two-variable difference equation, with these boundary conditions is

$$D_{a,b} = \frac{3}{n}ab(n - a - b).$$

This can be verified by substitution but that leaves open the question of how such a solution is obtained. To motivate the equation by guessing, note that the original problem is symmetric in the urns A, B and C, that is it does not matter which urn is labeled A. In turn, that means the solution must be symmetric in the variables  $a$  and  $b$ . Since the only symmetric polynomials in  $a$  and  $b$  are  $ab$  and  $a + b$ , it makes sense to search for a solution as a combination of these variables. Furthermore, the product  $Kab(n - a - b)$  (where  $K$  is a constant to be determined) satisfies the boundary conditions. Finally, this product is similar to the solution  $a(n - a)$  in the two urn, single variable case. Substituting  $Kab(n - a - b)$  and determining the constant  $K$  reveals the solution.

3.6: The equality is trivial for the base case  $m = 1$ . Assume the equality holds for  $m - 1$ . Check the multiplication for the lower left block, the other three

blocks are easily seen to hold. The multiplication for the lower left block is

$$((I_t + T + T^2 + \cdots + T^{m-2})A)I_a + T^{m-1}A = (I_t + T + T^2 + \cdots + T^{m-1})A.$$

Note  $AI_a = A$ . Using associative and distributive properties for matrix multiplication completes the induction step.

- 3.7: (a) With R, for  $p = 1/2$ ,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.924$ . With R, for  $p = 2/3$ ,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.933$ .  
 (b) With R,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.794$ .  
 (c) With R,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.866$ .  
 (d) Proof lightly adapted from StackExchange – Substochastic matrix spectral radius For any state  $i$  and integer  $n \geq 0$ , let  $r_i^n = \sum_{\nu} (T^n)_{i\nu}$  denote the  $i$ th row sum of  $T^n$ . For  $n = 1$ , for convenience write  $r_i$  rather than  $r_i^1$ . Since  $T$  is a substochastic transition probability matrix,  $0 \leq r_i^n \leq 1$ . Let  $l^*$  be an index with  $r_{l^*} < 1$ , and note that for  $n \geq 1$

$$r_{l^*}^n = \sum_l T_{l^*l} r_l^{n-1} \leq \sum_l T_{l^*l} = r_{l^*} < 1.$$

By irreducibility, for any  $i$ , there is an  $m$  with  $(T^m)_{il^*} > 0$ . In fact, if  $T$  is an  $N \times N$  matrix, and  $i \neq l^*$  then take  $m < N$ . (Take the shortest path from  $i$  to  $l^*$  with positive transition probability). Since  $(T^m)_{il}$  puts positive weight on the index  $l = l^*$ ,

$$r_i^N = \sum_l T_{il}^m r_l^{N-m} < r_i^m \leq 1.$$

That is, every row sum of  $T^N$  is strictly less than 1. Now it is possible to show  $T^{jN} \rightarrow 0$  as  $j \rightarrow \infty$  and this shows  $T^N$  (and hence  $T$ ) cannot have any eigenvalue with modulus 1.

- (e) Note that if  $\mathbf{x} = (0, 1, 0, 0)^T$ , then  $T\mathbf{x} = (0, 1, 1/2, 0)$  with  $\|T(x)\| = \sqrt{5}/2 \approx 1.118 > 1$ . In fact, With R,  $\text{norm}(T, \text{type}=\text{c}("2")) = 1.162$  but the eigenvalues are 0.833, 0.500, 0 and 0. The previous theorem is not violated because the transient transition probability matrix is not irreducible, it is not possible to reach state 1 + 1 + 1 + 1. Note also the converse of the previous theorem is not true: This matrix has operator norm less than 1, but it is not irreducible.

3.8: First note  $NT = TN$  because

$$\begin{aligned} T(I_t - T) &= (I_t - T)T \\ T &= (I_t - T)T(I_t - T)^{-1} \\ (I_t - T)^{-1}T &= T(I_t - T)^{-1} \\ NT &= TN \end{aligned}$$

Start with  $N = (I_t - T)^{-1}$ . Then

$$\begin{aligned}
 I_t &= N(I_t - T) \\
 0 &= N - NT - I_t \\
 T &= N - TN - I_t + T \\
 T &= (I_t - T)N - (I_t - T) \\
 T &= (I_t - T)(N - I_t) \\
 (I_t - T)^{-1}T &= N - I_t
 \end{aligned}$$

3.9: Consider

$$\begin{aligned}
 (I - T)(I + T + T^2 + \cdots + T^m) &= (I + T + T^2 + \cdots + T^m) - \\
 &\quad (T + T^2 + \cdots + T^{m+1}) = I - T^{m+1}
 \end{aligned}$$

Then

$$\|(I - T) \sum_{\nu=0}^m (T^\nu) - I\| = \|T^{m+1}\| \rightarrow 0$$

so

$$\sum_{\nu=0}^{\infty} (T^\nu) = (I - T)^{-1}.$$

3.10: With 1 candle, and the assumption you blow out a random number of candles between one and the number that remain,  $w_1$  must be  $1 = H_1$  and the base case is established. Next assume

$$w_N = H_N = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \cdots + \frac{1}{N} = \sum_{\nu=1}^N \frac{1}{\nu}.$$

The first-step equation is

$$\begin{aligned}
 w_{N+1} &= 1 + \frac{1}{N+1}w_1 + \frac{1}{N+1}w_2 + \cdots + \frac{1}{N+1}w_N \\
 &= 1 + \frac{1}{N+1} \sum_{\nu=1}^N w_\nu \\
 &= 1 + \frac{1}{N+1} \sum_{\nu=1}^{N+1} \sum_{j=1}^{\nu} \frac{1}{j} \\
 &= 1 + \frac{1}{N+1} \sum_{j=1}^N \frac{N - (j-1)}{j} \\
 &= 1 + \frac{1}{N+1} \sum_{j=1}^N \left( \frac{N+1}{j} - 1 \right) \\
 &= 1 + \sum_{j=1}^N \frac{1}{j} - \frac{1}{N+1}(N) \\
 &= \sum_{j=1}^N \frac{1}{j} + \frac{1}{N+1} \\
 &= w_{N+1}
 \end{aligned}$$

Chapter 4: Standard Examples.

4.1: (a) For the first Ehrenfest model

$$P_{ij} = \begin{cases} i/k & \text{if } j = i - 1, \\ (k-i)/k & \text{if } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$

(b) For the second Ehrenfest model

$$P_{ij} = \begin{cases} \frac{i}{k}q & \text{if } j = i - 1, \\ \frac{i}{k}p + \frac{k-i}{k}q & \text{if } j = i, \\ \frac{k-i}{k}p & \text{if } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$

(c) For the third Ehrenfest model

$$P_{ij} = \begin{cases} \frac{k-i}{k}p & \text{if } j = i - 1, \\ \frac{i}{k}p + \frac{k-i}{k}q & \text{if } j = i, \\ \frac{i}{k}q & \text{if } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$



(d) For the fourth Ehrenfest model

$$P_{ij} = \begin{cases} \frac{i(k-i)}{k^2} & \text{if } j = i - 1, \\ \frac{i^2}{k^2} + \frac{(k-i)^2}{k^2} & \text{if } j = i. \\ \frac{i(k-i)}{k^2} & \text{if } j = i + 1, \\ 0 & \text{otherwise.} \end{cases}$$

4.2: Entry  $i$  must satisfy

$$\binom{k}{i-1} \left(\frac{1}{2}\right)^k \cdot \frac{k-i+1}{k} + \binom{k}{i+1} \left(\frac{1}{2}\right)^k \cdot \frac{i+1}{k} = \binom{k}{i} \left(\frac{1}{2}\right)^k$$

or more simply

$$\binom{k}{i-1} \cdot \frac{k-i+1}{k} + \binom{k}{i+1} \cdot \frac{i+1}{k} = \binom{k}{i}.$$

This reduces to

$$\binom{k-1}{i-1} + \binom{k-1}{i+1} = \binom{k}{i}.$$

which is the basic binomial (Pascal triangle) identity.

4.3: Using the probability transition matrix from `ehrfest3.R` and using the `markovchain` package in R:

```
R> absorptionProbabilities(ehrenfest3)
      0      7
1 0.984375 0.015625
2 0.890625 0.109375
3 0.656250 0.343750
4 0.343750 0.656250
5 0.109375 0.890625
6 0.015625 0.984375
R> meanAbsorptionTime(ehrenfest3)
      1      2      3      4      5      6
3.033333 7.233333 10.733333 10.733333 7.233333 3.033333
```

Using the probability transition matrix from `ehrfest4.R` and using the `markovchain` package in R:

```
R> absorptionProbabilities(ehrenfest4)
      0      7
1 0.8571429 0.1428571
2 0.7142857 0.2857143
3 0.5714286 0.4285714
4 0.4285714 0.5714286
5 0.2857143 0.7142857
6 0.1428571 0.8571429
R> meanAbsorptionTime(ehrenfest4)
      1      2      3      4      5      6
17.15000 26.13333 30.21667 30.21667 26.13333 17.15000
```

4.4:

$$P = \begin{pmatrix} 1-p & p & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

and

$$(\pi_{1,0}, \pi_{0,1}, \pi_{0,2}) = \left( \frac{1}{1+2p}, \frac{p}{1+2p}, \frac{p}{1+2p} \right).$$

4.5: Let the state be the number  $i$  of white balls in the first urn. This determines the number of black balls in the first urn and the number of black and white balls in the second urn.  $p_{ii} = 2i(m-i)/m^2$ ,  $p_{i,i-1} = i^2/m^2$ ,  $p_{i,i+1} = (m-i)^2/m^2$ . After a large number of turns  $\pi_j = \binom{m}{k} \pi_0$ , where  $1/\pi_0 = \sum_{i=0}^m \left( \binom{m}{i} \right)^2 = \binom{2m}{m}$  and  $\pi_j = \left( \binom{m}{i} \right)^2 / \binom{2m}{m}$ .

4.6: The state space is the set of nonnegative integers. At time period  $t$ , suppose there are  $i$  infected individuals not in quarantine. Suppose that  $j$  ( $0 \leq j \leq i$ ) of these contagious individuals infect another  $j$  individuals and that  $i-j$  are discovered and moved to quarantine. At the next time period there are a net number  $i+j-(i-j) = 2j$  infectives in the population with probability  $\binom{i}{j} p^j (1-p)^{i-j}$ . This is a discrete time Markov chain on an infinite state space with transition probability  $p_{i\ell} = \binom{i}{\ell/2} p^{\ell/2} (1-p)^{i-(\ell/2)}$  for  $i \geq 0$  and  $0 \leq \ell \leq 2i$  and  $\ell$  even.

The probability that by period 1 the one carrier has not been discovered is  $p$ , by period 2 there are 2 carriers and the probability that each is not yet discovered is  $p^2$ , by period three there are 4 carries with no discoveries with probability  $p^4$ , and by period  $n$  there are  $2^{n-1}$  carriers with no discoveries  $p^{2^{n-1}}$ .

Chapter 5: The Game of Monopoly as a Markov Chain.

5.1: Use the following script:

```

1  library("markovchain")
2
3  rotvec <- function(vec) vec[ c(length(vec), 1:(length
4    (vec)-1)) ]
5
6  nStates <- 8
7  monopolyStates <- as.character( c(1:nStates) )
8
9  diceRoll <- matrix(0, nStates, nStates)
10 p1 <- c(0, 1/2, 1/2, 0, 0, 0, 0, 0)
11 for (i in 1:nStates) {
12   diceRoll[i, ] <- p1
13   p1 <- rotvec(p1)
14 }
15
16 Jail <- diag(nStates)
17 Jail[4, 4] <- 0
18 Jail[4, 2] <- 1                                #go from Police
                                           to Jail

```

```

19 |
20 | Ch <- diag(nStates)
21 | Ch[6, 7] <- 1/16                                #Nearest
      Railroad
22 | Ch[6, 8] <- 1/16                                #Advance to
      Go
23 | Ch[6, 1] <- 1/16                                #Reading
      Railroad
24 | Ch[6, 2] <- 1/16                                #Go to Jail
25 | Ch[6, 3] <- 1/16                                #Go back 3
26 | Ch[6, 6] <- 11/16                               #All other
      cards
27 |
28 | monopolMat <- diceRoll %*% Jail %*% Ch
29 |
30 | mcMonopoly8 <- new("markovchain", states =
      monopolyStates, byrow = TRUE,
31 |                   transitionMatrix = monopolMat, name =
      "Monopoly")
32 | ss <- steadyStates(mcMonopoly8)
33 | cat(ss, "\n")

```

```

      1 0.07731016
      2 0.383806
      3 0.2342177
The stationary distribution is 4 0.0
      5 0.1171089
      6 0.04025618
      7 0.08234218
      8 0.06495883

```

Chapter 6: The Game of Risk as a Markov Chain.

6.1: For  $Y^{(1)} = y^{(1)}$ ,  $Y^{(2)} = y^{(2)}$  with  $y^{(1)} > y^{(2)}$ , the individual die values *in some order* must be  $y^{(1)}$ ,  $y^{(2)}$  and  $y^{(3)} \leq y^{(2)}$ . There are 6 orders for each of the  $y^{(2)}$  possibilities for  $y^{(3)}$ , each with probability  $\frac{1}{6^3}$ . However, if  $y^{(3)} = y^{(2)}$ , then the 6 orders are counted twice, so half of them, specifically 3, must be subtracted from the total.

6.2: Count the ways it is possible to have  $Y^{(1)} = y^{(1)}$ . There is 1 way to have  $y^{(1)} = Y^{(1)} = Y^{(2)} = Y^{(3)}$ . There are  $y^{(1)} - 1$  ways to have  $y^{(1)} = Y^{(1)} = Y^{(2)} > Y^{(3)}$  in 3 possible permutations each. There are  $(y^{(1)} - 1)(y^{(1)} - 2)$  ways to have  $y^{(1)} = Y^{(1)} > Y^{(2)} > Y^{(3)}$  in 6 possible permutations each. Each way has probability  $\frac{1}{216}$  so after expanding and simplifying

$$\mathbb{P}[Y^{(1)} = y^{(1)}] = \frac{1 - 3y^{(1)} + 3(y^{(1)})^2}{216}$$

for  $y^{(1)} = 1, 2, 3, 4, 5, 6$ .

6.3: Use the order statistic probability

$$\mathbb{P}[Y^{(1)} = y^{(1)}] = (1 - 3y^{(1)} + 3(y^{(1)})^2)/216.$$

The possibilities for the defender to lose one army are the following:

- (a) The largest die of the 3 rolled by the attacker is a 2, and the value rolled by the defender is 1; occurring with probability  $\frac{7}{216} \cdot \frac{1}{6} = \frac{7}{1296}$ .
- (b) The largest die of the 3 rolled by the attacker is a 3, and the value rolled by the defender is 1 or 2; occurring with probability  $\frac{19}{216} \cdot \frac{2}{6} = \frac{38}{1296}$ .
- (c) The largest die of the 3 rolled by the attacker is a 4, and the value rolled by the defender is 1 or 2 or 3; occurring with probability  $\frac{37}{216} \cdot \frac{3}{6} = \frac{111}{1296}$ .
- (d) The largest die of the 3 rolled by the attacker is a 5, and the value rolled by the defender is 1, 2, 3, or 4; occurring with probability  $\frac{61}{216} \cdot \frac{4}{6} = \frac{244}{1296}$ .
- (e) The largest die of the 3 rolled by the attacker is a 6, and the value rolled by the defender is 1, 2, 3, 4, or 5; occurring with probability  $\frac{91}{216} \cdot \frac{5}{6} = \frac{455}{1296}$ .
- (f) The total probability is  $(7+38+111+244+455)/1296 = 855/1296$  (which reduces to  $95/144$ ).

	20	19	18	17	16
	4.441	4.277	4.111	3.943	3.773
	15	14	13	12	11
6.4:	3.601	3.427	3.249	3.068	2.883
	10	9	8	7	6
	2.692	2.498	2.293	2.085	1.854
	5	4	3	2	1
	1.631	1.335	1.110	0.590	0.417

Chapter 7: Games.

7.1: The transition probability matrix for *Tenzi* (rounded to three decimal places) is written in Maxima as

```

pi[i,j] := if (j >= i) then binomial(11-i, j-i) * ((1/6)^(j-i)) *
((5/6)^(11-j)) else 0;
P : genmatrix(pi, 11, 11);
fpprintprec : 3;
float(P);

```

Transfer this matrix of values to R and evaluate with the following script:

```

x <- c(0.1615055828898457, 0.3230111657796915, 0.2907100492017223,
0.1550453595742519, 0.05426587585098816, 0.01302381020423716,
0.002170635034039527, 2.48072575318803*10^-4,
1.860544314891023*10^-5, 8.2690858439601*10^-7,
1.65381716879202*10^-8, 0.0, 0.1938066994678149,
0.3488520590420667, 0.2790816472336534, 0.1302381020423716,
0.03907143061271148, 0.007814286122542296,
0.001041904816338973, 8.930612711476907*10^-5,
4.465306355738455*10^-6, 9.922903012752121*10^-8, 0.0, 0.0,
0.2325680393613778, 0.3721088629782046, 0.2604762040847432,
0.1041904816338973, 0.02604762040847432, 0.004167619265355891,
4.167619265355891*10^-4, 2.381496723060509*10^-5,

```

```

5.953741807651273*10^-7,0.0, 0.0, 0.0, 0.2790816472336534,
0.3907143061271148, 0.2344285836762689, 0.07814286122542295,
0.01562857224508459, 0.001875428669410151,
1.250285779606767*10^-4, 3.572245084590763*10^-6,0.0, 0.0,
0.0, 0.0, 0.3348979766803841, 0.4018775720164609,
0.2009387860082305, 0.05358367626886145, 0.008037551440329218,
6.430041152263375*10^-4, 2.143347050754458*10^-5,0.0, 0.0,
0.0, 0.0, 0.0, 0.4018775720164609, 0.4018775720164609,
0.1607510288065844, 0.03215020576131687, 0.003215020576131687,
1.286008230452675*10^-4,0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.4822530864197531, 0.3858024691358025, 0.1157407407407407,
0.0154320987654321, 7.716049382716049*10^-4,0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.5787037037037037, 0.3472222222222222,
0.06944444444444445, 0.004629629629629629,0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.6944444444444444, 0.2777777777777778,
0.0277777777777778,0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.0, 0.8333333333333334, 0.1666666666666667,0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0)
P <- t( matrix(x, 11, 11) )

PPow <- P
tenzicdf <- c(PPow[1,11])
for (i in 2:50) {
  PPow <- PPow %*% P;
  tenzicdf <- c(tenzicdf, PPow[1,11])
}

library(ggplot2)
ggplot(data = as.data.frame(tenzicdf), aes(x=1:50, y=tenzicdf))
+ geom_point()
+ geom_line()

tenzipdf <- tenzipdf[2:50] - tenzipdf[1:49]
tenzipdf <- c(tenzicdf[1], tenzipdf)
ggplot(data = as.data.frame(tenzipdf), aes(x=1:50, y=tenzipdf))
+ geom_point()
+ geom_line()

sum(tenzipdf)
tenzimean <- (1:50) %*% tenzipdf

Q <- P[1:10, 1:10]
I10 <- ident(10)
N <- solve( I10 - Q, I10)
N %*% rep(1,10)

Varw <- ((2 * N - I10) %*% N) %*% rep(1, 10) - ( N %*% rep(1, 10) )^2

```

```
sdw <- sqrt(Varw)
```

7.2: (1) Denote as  $P(n, j)$  the probability that the minimum value from  $n$  random samples of  $p(j)$  is less than or equal to  $j$ . Then  $P(n, j)$  is the complement of the probability that all  $n$  random samples (which are independent of each other) are greater than  $j$ , so  $P(n, j) = 1 - (1 - P(j))^n$ . The p.d.f. giving the probability that a game with  $n$  players is won in exactly  $j$  rolls is  $p(n, j) = P(n, j) - P(n, j - 1)$ .

(2) The expected number of turns in a game of Tenzi with 2 players is 11.897, with 3 players is 10.408, and with 4 players is 9.542.

7.3: A possible path is to roll a 1, to 38; roll a 6, to 44; roll a 6, to 50; roll a 1, to 67; roll a 6, to 73; roll a 6, to 79 and finally, roll a 1 to ascend from 80 to 100. Examination of the first 6 powers of the transition probability matrix show that the probability of 6 step paths from 38 is 0.007265947 but 0 for fewer than 6 steps.

Another possible path is roll a 4, to 14; roll a 6, to 20; roll a 6, to 26; roll a 2, to 84; roll a 6, to 90; roll a 5, to 75 and finally, roll a 5 to ascend from 80 to 100. Examination of the first 6 powers of the transition probability matrix show that the probability of 6 step paths from 14 is 0.001800412 but 0 for fewer than 6 steps.

7.4: (a) The expected length of a game with no chutes or ladders is 31.1 with a standard deviation of 5.98.

(b) The expected length of the game drops from about 39.2 to about 29.8 with a standard deviation of about 18.8.

(c) The game lengthens to about 45.8 moves with a standard deviation of about 33.4.

(d) Lengthens the expected playing time by more than two moves to about 41.9, since it increases the chances of missing the important ladder from state 80 to 100.

(e) Shortens the game by over a move to about 38.0, since it gives a second chance at the long ladder from 28 to 84.

7.5: The win probability if only square 2 is blue is 0.5288 The win probability if squares 2, 3 and 5 are blue is 0.7761. The remaining questions make a good project for student investigation.

7.6: First build some general Julia code to create the transition probability matrices for any  $n$ . This general code does not need the specialized Markov chain packages, but does use the **Graphs** package to check for dominance cycles.

```
1 function markov(size::Integer)
2     idx2states = vec(join.(Iterators.product([ 'h', 't' ] for _ in 1:size)...))
3     states2idx = Dict{idx2states => eachindex(idx2states)}
4     P = zeros(2^size, 2^size)
5     for state in idx2states
6         for next in ("h", "t")
7             nextstate = chop(state, head=1, tail=0) *
            next
```

```

8           P[states2idx[state], states2idx[nextstate]
9       ]] = 0.5
10         end
11     end
12     return P, idx2states, states2idx
end

```

- (1) The `idx2states` vector keeps track of all H and T sequences that have length  $n$  (i.e. it is a mapping from state number to state signature).
- (2) `states2idx` is an inverse mapping from state signature to state number.
- (3) `P` is the transition probability matrix of the chain. Note that from the sequence AB ... (where all elements are H or T) we go to sequence B ...H or B dots T with equal probability.

Next some general code to make Alice and Bob's chosen sequences the absorbing states for game. Instead of rearranging to canonical form and finding the absorption probabilities, make  $2^{32}$  steps of the process (fortunately in Julia it is fast by 5 matrix squarings). Observe that initially all states are equally probably, so the `terminal` matrix keeps information about long term probabilities of staying in all possible states.

```

1 function game(P, states2idx, alice, bob)
2     P_game = copy(P)
3     alice_idx, bob_idx = states2idx[alice],
4     states2idx[bob]
5     P_game[alice_idx, :] .= 0.0
6     P_game[alice_idx, alice_idx] = 1.0
7     P_game[bob_idx, :] .= 0.0
8     P_game[bob_idx, bob_idx] = 1.0
9     n = length(states2idx)
10    terminal = fill(1 / n, 1, n) * P_game^(2^32)
11    return terminal[states2idx[alice]], terminal[
12    states2idx[bob]]
end

```

Finally some code to analyze the game.

```

1     using Graphs
2
3 function analyze_game(size::Integer, details::Bool=
4     true)
5     P, idx2states, states2idx = markov(size)
6     g = SimpleDiGraph(length(states2idx))
7     details && println("\nWinners:")
8     for alice in idx2states, bob in idx2states
9         alice > bob || continue

```

```

9      alice_win, bob_win = game(P, states2idx,
alice, bob)
10     if alice_win > 0.51
11         winner = "alice"
12         add_edge!(g, states2idx[alice],
states2idx[bob])
13     elseif bob_win > 0.51
14         winner = "bob"
15         add_edge!(g, states2idx[bob], states2idx[
alice])
16     else
17         winner = "tie (or close)"
18     end
19     details && println(alice, " vs ", bob, ": ",
winner)
20 end
21 cycles = simplecycles(g)
22 if !isempty(cycles)
23     min_len = minimum(length, cycles)
24     filter!(x -> length(x) == min_len, cycles)
25 end
26 println("\nCycles:")
27 for cycle in cycles
28     println(idx2states[cycle])
29 end
30 end

```

```

(1)
1     game2 = markov(2)
2     P = game2[1]
3     game(P, states2idx, "th", "hh")
4     game(P, states2idx, "th", "hh")
5

```

Alice wins with probability 0.75, Bob wins with probability 0.25.

```

(2)
1     game3 = markov(3)
2     P = game3[1]
3     states2idx = game3[3]
4     game(P, states2idx, "tth", "hhh")
5

```

Alice wins with probability 0.7, Bob wins with probability 0.3.

(3) `analyze_game(3)` The shortest cycle has length 4 and it is unique.



```

Winners:
thh vs hhh: alice
thh vs hth: tie (or close)
thh vs hht: alice
thh vs htt: tie (or close)
hth vs hhh: alice
hth vs hht: bob
tth vs hhh: alice
tth vs thh: alice
tth vs hth: alice
tth vs hht: tie (or close)
tth vs tth: alice
tth vs htt: bob
hht vs hhh: tie (or close)
tth vs hhh: alice
tth vs thh: tie (or close)
tth vs hth: tie (or close)
tth vs hht: bob
tth vs htt: tie (or close)
htt vs hhh: alice
htt vs hth: tie (or close)
htt vs hht: bob
htt vs htt: tie (or close)
ttt vs hhh: tie (or close)
ttt vs thh: bob
ttt vs hth: bob
ttt vs tth: tie (or close)
ttt vs hht: bob
ttt vs tth: bob
ttt vs htt: bob

```

```

Cycles:
["thh", "hht", "htt", "tth"]

```

- (4) `analyze_game(4, false)` shows 14 cycles of length 3, shorter than the unique cycle for  $n = 3$ !

This problem and the code for the solution is from <https://bkamins.github.io/julialang/2024/06/14/probability>

- 7.7: (a) For this question, the rounds don't matter at all. The game will end once there is at least 1 correct ball in each cup, and the pruning phase at the end of each round only removes incorrect balls so effectively neglects pruning.

This is a classical coupon collector problem. Define  $Y_i$ , for  $i$  from 0 to  $N - 1$ , to be the number of additional tosses that need to be obtained after  $i$  distinct cups have been filled with corresponding numbered balls. Define  $Y$  as the total number of tosses required to fill the cups with correspondingly numbered balls so

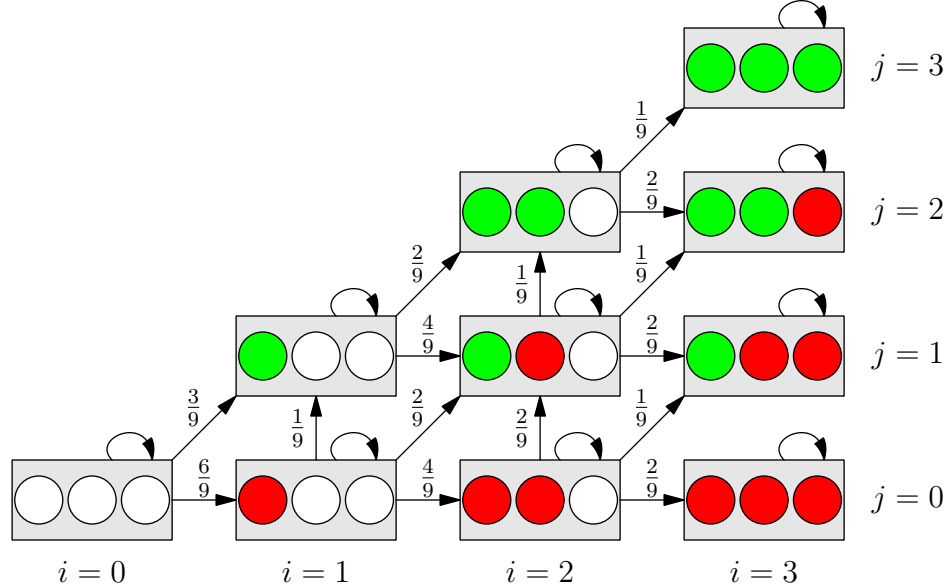
$$Y = Y_0 + Y_1 + Y_2 + \cdots + Y_{N-1}.$$

When  $i$  distinct cups have been filled with corresponding numbered balls, the probability that a ball with a number of an unfilled cup is drawn is  $\frac{N-i}{N}$ . Each time a ball is thrown, there is a  $1/N$  chance it will land in the correct cup. It follows that the probability of success in filling a new cup with the correctly numbered ball is  $\frac{N-i}{N} \cdot \frac{1}{N}$ . Thus,  $Y_i$  is a geometric random variable with success parameter  $\frac{N-i}{N^2}$ . Then  $\mathbb{E}[Y_i] = \frac{N^2}{N-i}$ . Therefore

$$\begin{aligned}\mathbb{E}[Y] &= \mathbb{E}[Y_0] + \mathbb{E}[Y_1] + \mathbb{E}[Y_2] + \cdots + Y_{N-1} \\ &= N + \frac{N^2}{N-1} + \frac{N^2}{N-2} + \cdots + \frac{N^2}{1} \\ &= N^2 \sum_{\nu=1}^N \frac{1}{\nu} \approx N^2(\log N + \gamma)\end{aligned}$$

where  $\gamma \approx 0.577$  is the Euler-Mascheroni constant.

- (b) In general the number of rounds to end the game is complicated, so to illustrate the approach solve it for the case  $N = 3$ . Begin by breaking each round into a number of stages. Each stage tracks the progress of cups as they are filled. In the diagram below, each cup is either empty (no ball), is red (incorrect ball), or is green (correct ball). The transition probabilities are on the arrows.



The integer  $i$  indicates the number of balls thrown. The integer  $j$  indicates the number of cups filled holding a correspondingly numbered ball. A colored cup may contain more than 1 ball. The cup position left to right is not associated with the cup or ball numbers, the position merely indicates the number of correctly or incorrectly filled cups. For example, if 2 balls have been thrown into 2 cups, 1 correctly numbered, 1 incorrectly numbered, the center diagram at  $i = 2, j = 1$  illustrates this case. Then

on the next ball thrown, that ball can incorrectly go into the empty cup with probability  $\frac{N-1}{N} \cdot \frac{1}{N} = \frac{2}{9}$ . The ball can go into the correct cup with probability  $\frac{1}{N}$ . In this diagram, self-loops have whatever probability is required so that the outgoing arrows sum to 1. This is a Markov chain. Start on the initial state at the lower left (all cups empty,  $i = 0, j = 0$ ), and advance to an absorbing state at the right, all cups full with  $i = 3$ . Label the states by columns from top to bottom from right to left. This unusual ordering puts the transition matrix in canonical form. The transition matrix for  $N = 3$  is:

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{9} & \frac{2}{9} & 0 & 0 & \frac{6}{9} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{9} & \frac{2}{9} & 0 & \frac{1}{9} & \frac{5}{9} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{9} & \frac{2}{9} & 0 & \frac{2}{9} & \frac{4}{9} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{9} & \frac{4}{9} & 0 & \frac{3}{9} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{9} & \frac{4}{9} & \frac{1}{9} & \frac{2}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{9} & \frac{6}{9} & 0 \end{pmatrix}.$$

The matrix  $N = (I - T)^{-1}$  is:

$$N = \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 3 & 9 & 0 & 0 & 0 & 0 \\ 3 & 4 & 0 & 0 & 0 & 0 \\ 3 & 9 & 0 & 0 & 0 & 0 \\ 3 & 10 & 0 & 0 & 0 & 0 \\ 3 & 3 & 0 & 3 & 0 & 0 \\ 1 & 3 & 0 & 3 & 9 & 0 \\ 37 & 48 & 36 & 3 & 9 & 0 \\ 35 & 35 & 35 & 14 & 6 & 0 \\ 48 & 99 & 34 & 9 & 6 & 1 \\ 35 & 70 & 35 & 14 & 7 & 1 \end{pmatrix}$$

and

$$B = NA = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 & 0 \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{2} & 0 \\ \frac{1}{12} & \frac{1}{12} & \frac{2}{5} & \frac{2}{5} \\ \frac{1}{30} & \frac{1}{6} & \frac{1}{5} & 0 \\ \frac{1}{6} & \frac{1}{2} & \frac{3}{4} & 0 \\ \frac{1}{15} & \frac{2}{7} & \frac{10}{5} & \frac{8}{35} \\ \frac{1}{10} & \frac{1}{14} & \frac{41}{105} & \frac{16}{105} \end{pmatrix}.$$

The  $ij$  entry in  $B$  gives the probability of going from state  $i+4$  to absorbing state  $j = 1, 2, 3, 4$ .

Being in absorbing state  $j$  means the throwing phase of the round ends and the pruning phase of the round begins. Absorbing state 1 requires no pruning, the round is finished. Absorbing state 2 transitions to state 5, state 3 transitions to state 8 and state 4 transitions to state 10 and the throwing part of the next round resumes.

Now let  $E_5, E_8, E_{10}$  be the expected number of rounds played to end the game starting from states 5, 8, 10 respectively. The main interest is  $E_{10}$  which answers the question. Using first-step analysis, these expected

	<i>AB</i>	<i>S</i>	<i>D</i>	<i>T</i>	<i>HR</i>	<i>BB</i>	<i>AVE</i>	<i>SA</i>	<i>OB</i>	<i>OPS</i>
Ruth	8399	1517	506	136	714	2062	0.342	0.690	0.474	1.164
Williams	7706	1537	525	71	521	2021	0.344	0.634	0.481	1.114

**Table 21.1.** Statistics for Babe Ruth and Ted Williams.

values satisfy the equations

$$\begin{aligned}
 E_5 &= 1 + \frac{2}{3}E_5 \\
 E_8 + 1 + \frac{1}{2}E_5 + \frac{1}{3}E_8 \\
 E_{10} &= 1 + \frac{5}{14}E_5 + \frac{41}{105}E_8 + \frac{16}{105}E_{10}.
 \end{aligned}$$

Solving numerically,  $E_5 = 3$ ,  $E_8 = 3.75$ ,  $E_{10} = 4.171$ .

This problem and the solution as a Markov chain appeared in FiveThirtyEight Riddler column of November 16, 2018. The solution and solution figures are adapted from Five Thirty Eight Riddler.

Chapter 8: A Markov Chain Model of Baseball.

8.1: In 2019, Strasburg was a pitcher for the Washington Nationals in the National League, as he had been since 2010. As a pitcher, his hitting skills and run production are not emphasized, it is his pitching that makes him a valuable player. Furthermore, as a pitcher, he appears in fewer games with even fewer plate appearances. That means he has a smaller base of hitting statistics for creating the matrix  $P$  so  $P$  may not fully reflect his hitting skills.

8.2: Using the script with Trout's statistics, the expected time to absorption starting from the first state of no-outs is 5.22 at-bats per half-inning.

8.3: In the  $25 \times 25$  matrix  $P_K$ , all entries are 0 except for the following:

- For each  $i$ ,  $i = 1, \dots, 25$  and  $j = 1, 2, 3$  with  $j = i \bmod 3$ ,  $(P_K)_{ij} = q$ ,
- For each  $i$ ,  $i = 1, \dots, 25$  with  $i \neq 0 \bmod 3$ , and  $j = i + 1$   $(P_K)_{ij} = 1 - q$
- For each  $i$ ,  $i = 1, \dots, 25$  with  $i = 0 \bmod 3$  and  $j = 25$   $(P_K)_{ij} = 1 - q$ .

In the special case  $q = 0.1$ , the Markov runs statistic for a half-inning is 0.333 and the markov RPG is 3.

8.4: Using the 2024 data for Aaron Judge, 2024 American League MVP, his markovRPG is 11.8.

8.5: The lifetime career statistics for Babe Ruth (1914–1935) and Ted Williams (1939–1942, 1946–1960) are in Table 0.3. (Values derived from Baseball-Reference.) Then

$$\rho_{BR} = (0.528, 0.197, 0.145, 0.048, 0.13, 0.068)$$

and

$$\rho_{TW} = (0.568, 0.212, 0.158, 0.054, 0.007, 0.054).$$

Using these probabilities in the script for Markov runs, the markov RPG for Babe Ruth is 12.65 and the value for Ted Williams is 12.55. The two values are close but Ruth has the slightly greater value.

No statistic can resolve the comparison between these two great players. Each played in different baseball eras, and each had particular strengths. Besides, what is to be the basis for comparison, their lifetime statistics used here, or the best career year for each? If the latter, how to choose the best career year? Note that Williams lost 3 (possibly best) years of his career to military service in World War II. It is interesting to compute the Markov runs for each, but the statistic won't answer this opinion question.

Chapter 9: Modeling Sports with Markov Chains.

9.1: Label the transient states in Figure 9.1 from 1 for 0:0 from to bottom, left to right and label the absorbing states last. Then 0:0 is state 1, state 40:30 is state 13, state 30:40 is state 15. The absorbing state "A wins" is 17 and "B wins" is 16. Use the script with this labeling.

For  $p = 0.6$ , the probability A wins is 0.736. For  $p = 0.6$ , the expected number of serves or points until absorption, that is the game ends, is 6.48 with a standard deviation of 2.59.

For  $p = 0.51$ , the probability A wins is 0.525. For  $p = 0.51$ , the expected number of serves or points until absorption, that is the game ends, is 6.75, only slightly longer. The standard deviation is 2.77, also slightly more.

The conclusion is that most games last between 4 and 9 serves, even if the players are nearly evenly matched. This makes sense, the game reaches the bottom row in 4 to 6 steps in any case and then is in the absorbing walk for a few steps.

9.2: Using a program script,

```
Mean A Scores:  90.14 Standard Deviation:  6.71
Mean B Scores: 100.64 Standard Deviation:  7.15
```

Chapter 10: Markov Chain Epidemic Models.

10.1: There is 1 state with  $S_t + I_t = 0$ , and 2 states with  $S_t + I_t = 1$ , namely  $S_t = 1$  with  $I_t = 0$  and  $S_t = 0$  with  $I_t = 1$ . Likewise there are  $i + 1$  states with  $S_t + I_t = i$  up to  $i = N$ . Then there are  $1 + 2 + \cdots + N + 1 = (N + 1)(N + 2)/2$  possible states.

10.2: The following script is a simple implementation of an epidemic on a two-dimensional grid. For a given value of  $N$ , the script defines a population of Susceptibles on a square grid of size  $2N + 1$ , and sets an Infective at the center location  $(N, N)$ . The infective can infect neighbors with probability  $p$ , and fails to infect neighbors with probability  $1 - p$ . Because the infection can only spread to immediate neighbors, the epidemic spreads through concentric rings of squares outward from the center. The spread in concentric rings means that the epidemic will take place over  $N$  steps, possibly stopping at some earlier step due to no Infectives, which the script reports. At each step, for all Infectives in the grid, the script successively infects immediate neighbors to the north, east, west and south with probability  $p$ . After possibly infecting neighbors, the infective becomes a Removed individual, so the infectious period lasts one step. At the end of each step, the script records the state of the epidemic. For testing and debugging, a value of  $N = 3$  is convenient. For an experiment, a value of  $N = 25$  is useful.

```

149 N <- 25
150 # N <- 3
151 p <- 0.6
152
153 popn <- matrix("S", 2*N+1, 2*N+1)
154 popn[N+1,N+1] <- "I"
155
156 dir <- list("N" = -1, "E" = 2*N+1, "S" = 1, "W" =
      -(2*N+1))
157
158 infect <- function(pos, d) {
159   if (popn[pos + d] == "S") {
160     if (runif(1) < p ){ popn[pos + d] <- "I"}
161   }
162 }
163
164 epidemic <- array("", dim=c(2*N+1, 2*N+1, N))
165
166 for (t in 1:N) { # RINGS or EPOCHS
167
168   infs <- which(popn == "I")
169   if (length(infs) == 0) {
170     cat("Epidemic ended after", t-1, "steps.\n")
171     break}
172   else {
173     for (j in infs) {
174       for (d in dir) {
175         infect(j, d)
176       }
177       popn[j] <- "R"
178     }
179     epidemic[, , t] <- popn
180   }
181 }
182
183 # # Animation code is adapted from
184 # # https://ryouready.wordpress.com/2010/11/21/
185 # # animate-gif-images-in-r-imagemagick/
186 # epidemicfactors <- array(as.numeric(factor(epidemic
187 #   )), dim=c(2*N+1, 2*N+1, N))
188 # par(xaxt="n", yaxt="n") #remove axis labels
189 #   and ticks
190 # png(file="epidemicImage%02d.png")
191 # for (t in 1:N) {
192 #   image(epidemicfactors[ , , t], col=c( "red", "
193 #     blue", "green" ))

```

```

190 # }
191 # dev.off()
192 # system("convert -delay 80 *.png epidemicAnimation.
      gif")
193
194 # file.remove(list.files(pattern=".png"))
      . language=R

```

This script is a very simple epidemic model with only basic attempts at efficiency. Many modifications are possible.

The animation is simple, relying on the graphics manipulation tool ImageMagick. The animation code is commented out because of the reliance on system dependent features. More elaborate animations are possible with other R packages such as plotly and gganimate.

Chapter 11: Reversible Markov Chains.

11.1: There are 6 detailed balance equations to check:

$$\begin{aligned}
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{1}{5} \cdot \frac{1}{2} \\
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{1}{5} \cdot \frac{1}{2} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{1}{5} \cdot \frac{1}{2} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{1}{5} \cdot \frac{1}{2}
 \end{aligned}$$

All are true, so the chain is reversible. Actually, only the first 3 equations need to be checked, since the last three are just the first three reversed.

11.2: Use the detailed balance to obtain  $\pi_1 P_{14} = \pi_4 P_{41}$  and  $\pi_1 P_{13} = \pi_3 P_{31}$  and  $\pi_3 P_{32} = \pi_2 P_{23}$  so  $\pi_1(1/2) = \pi_4(1/2)$  and  $\pi_1(3/40) = \pi_3(3/10)$  and  $\pi_3(1/4) = \pi_2(1/4)$ . Hence  $\pi_2 = \pi_3 = \pi_1/4 = \pi_4/4$ . Since the sum of the probabilities is 1,  $\pi_1 = \pi_4 = 4/10 = 2/5$  and  $\pi_2 = \pi_3 = 1/10$ .

11.3: This Markov chain has a stationary distribution

$$\pi = \left( \frac{1}{11}, \frac{4}{33}, \frac{1}{11}, \frac{4}{33}, \frac{5}{33}, \frac{4}{33}, \frac{1}{11}, \frac{4}{33}, \frac{1}{11} \right).$$

11.4: (a) The king makes a random walk on a graph with 32 vertices (the black squares) with degrees 1 on 2 corner squares, 2 on 12 side squares, and 4 on 18 interior squares. For a corner square  $i$ ,  $\pi_i = \frac{1}{1 \cdot 2 + 2 \cdot 12 + 4 \cdot 18} = \frac{1}{98}$  so the answer is 98.

(b) Label one corner starting square as state 1 and the other corner starting square as state 32. The stationary probability of occupying state 1 is  $\pi_1 = \frac{1}{98}$  and the stationary probability of occupying state 32 is also  $\pi_1 = \frac{1}{98}$ . Since the walks are independent processes, the joint probability of

occupying both states simultaneously is  $\pi_1 \pi_{32} = \frac{1}{98^2}$  and the expected number of steps is  $98^2$ .

11.5: For general  $n \geq 5$ , it is necessary to check each loop of length 3, of which there are  $\binom{n}{3}$ , and once those 3 states chosen, there is only one way to write the criterion equation. Then the number of 3 state loops can be written as  $\binom{n}{3}(3-1)!/2$ .

For the loops over 4 states, there are  $\binom{n}{4}$  choices of states. For the chosen set of 4, fix the starting state and there are  $3!$  orders for the remaining states. However, since the other side of the equation is the reversed path, there are only  $3!/2$  distinct paths of 4 states with the first state fixed.

For the loops over 5 states, there are  $\binom{n}{5}$  choices of states. For the chosen set of 5, fix the starting state and there are  $4!$  orders for the remaining states. However, since the other side of the equation is the reversed path, there are only  $4!/2$  distinct paths of 5 states with the first state fixed.

The same argument continues for general  $n \geq 5$ .

11.6: Suppose the Markov chain has a state  $j_{(*)}$  with  $P_{ij_{(*)}} > 0$  and  $P_{j_{(*)}i} > 0$  for  $1 < i < k$ . The goal is to show the Markov chain is reversible if and only if

$$P_{j_{(*)},j_1} P_{j_1,j_2} P_{j_2,j_{(*)}} = P_{j_{(*)},j_2} P_{j_2,j_1} P_{j_1,j_{(*)}}$$

for all  $1 < j_1, j_2 < k$ . Then

$$P_{j_1 j_2} = \frac{P_{j_{(*)} j_2}}{P_{j_{(*)} j_1}} P_{j_2 j_1} \frac{P_{j_1 j_{(*)}}}{P_{j_2 j_{(*)}}}.$$

This rewritten equality uses the hypothesis that  $P_{ij_{(*)}} > 0$  and  $P_{j_{(*)}i} > 0$ . Start with the loop probability

$$P_{j_0 j_1} P_{j_1 j_2} \cdots P_{j_{\ell-1} j_\ell} P_{j_\ell j_0}$$

and substitute the rewritten three step equality to obtain

$$\frac{P_{j_{(*)} j_1}}{P_{j_{(*)} j_0}} P_{j_1 j_0} \frac{P_{j_0 j_{(*)}}}{P_{j_1 j_{(*)}}} \frac{P_{j_{(*)} j_2}}{P_{j_{(*)} j_1}} P_{j_2 j_1} \frac{P_{j_1 j_{(*)}}}{P_{j_2 j_{(*)}}} \cdots \frac{P_{j_{(*)} j_\ell}}{P_{j_{(*)} j_{\ell-1}}} P_{j_\ell j_{\ell-1}} \frac{P_{j_{\ell-1} j_{(*)}}}{P_{j_\ell j_{(*)}}} \frac{P_{j_{(*)} j_0}}{P_{j_{(*)} j_\ell}} P_{j_0 j_\ell} \frac{P_{j_\ell j_{(*)}}}{P_{j_0 j_{(*)}}}.$$

Many terms cancel in a telescoping fashion, and reversing the order of multiplication gives the right side of the Kolmogorov loop criterion.

Brill et al. say Kelly *Reversibility and Stochastic Networks*, 1978, Cambridge University Press, Exercise 1.5.2, says that if there is a state which can be accessed *from* every other state in exactly 1 step, i.e. a column of the transition matrix has nonzero entries, then it is sufficient to check loops of only 3 states. However, neither source provides the proof, so it is possible that the exercise is mistaken. No counterexample is provided here, so the less restrictive criterion remains open here.

Chapter 12: Lumped Markov Chains.



12.1: To conform to the theorem, reorder the states to  $s_1, s_5, s_2, s_4, s_3$  so

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

Since this is an absorbing, not an irreducible and aperiodic, chain, applying the observation that all that is needed for  $U$  is that the  $i$ th row should be a probability vector with nonzero components only for states in  $E_i$

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

and

$$V = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then

$$VUPV = PV = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ 1/2 & 0 & 1/2 \\ 0 & 10 & 0 \end{pmatrix}$$

so the absorbing random walk is lumpable.

First calculate all the quantities for the original random walk.

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

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

$$N = (I_3 - Q)^{-1} = \begin{pmatrix} 3/2 & 1/2 & 1 \\ 1/2 & 3/2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

$$\mathbf{w} = N\mathbf{1} = (3, 3, 4)^T$$

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

Next calculate the absorption quantities for the lumped chain from the original chain using the submatrices  $U_A, U_T, V_A, V_T$  of  $U, V$ .

$$\begin{aligned}\hat{P} &= \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \end{pmatrix}, \\ \hat{N} &= U_T N V_T = \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix}, \\ \hat{\mathbf{w}} \hat{N} \mathbf{1} &= (3, 4)^T, \\ \hat{B} &= U_T B V_A = (1, 1)^T.\end{aligned}$$

Finally calculate the absorption quantities from the lumped chain canonical  $\hat{P}$  directly.

$$\begin{aligned}\hat{Q} &= \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \end{pmatrix}, \hat{R} = (1/2, 0)^T, \\ \hat{N} &= (I_T - \hat{Q})^{-1} = \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix}, \\ \hat{\mathbf{w}} &= \hat{N} \mathbf{1} = (3, 4)^T, \\ \hat{B} &= \hat{N} \hat{R} = (1, 1)^T.\end{aligned}$$

Both calculations of the absorption quantities agree.

12.2: On the left side

$$U_{ij} = \begin{cases} \pi_j / \sum_{x_\nu \in E_i} \pi_\nu & x_j \in E_i \\ 0 & \text{otherwise.} \end{cases}$$

On the right side,  $V_{ji} = 1$  if  $x_j \in E_i$  and 0 otherwise. Because  $\hat{\pi} = \pi V$ ,  $\hat{\pi}_i = \sum_{x_\nu \in E_i} \pi_\nu$ . Then the terms on the right side correspond precisely to the terms on the left side.

12.3: As a weighted random walk on a graph, the lazy random walk as a Markov chain is irreducible and reversible. For a hypercube of dimension  $k$ , the number of edges from each vertex is the dimension of the hypercube  $k$ , and the total number of vertices is  $2^k$ . The lazy random walk is associated with the weighted graph with self-edges with weight  $w_{ii} = k$  and  $k$  edges each with weight  $w_{ij} = 1$ . The sum of all weights from the  $2^k$  nodes is

$$s = \sum_{i,j} w_{ij} = (2k) \cdot 2^k.$$

The section on Reversible Markov Chains shows the invariant distribution is

$$\pi_i = \frac{2k}{(2k) \cdot 2^n} = \frac{1}{2^n}.$$

12.4: Entry  $i$  must satisfy

$$\binom{k}{i-1} \left(\frac{1}{2}\right)^k \cdot \frac{k-i+1}{2k} + \binom{k}{i} \left(\frac{1}{2}\right)^k \cdot \frac{1}{2} + \binom{k}{i+1} \left(\frac{1}{2}\right)^k \cdot \frac{i+1}{2k} = \binom{k}{i} \left(\frac{1}{2}\right)^k$$

or more simply

$$\binom{k}{i-1} \cdot \frac{k-i+1}{2k} + \binom{k}{i} \cdot \frac{1}{2} + \binom{k}{i+1} \cdot \frac{i+1}{2k} = \binom{k}{i}.$$

This reduces to

$$\binom{k-1}{i-1} + \binom{k-1}{i+1} = \binom{k}{i},$$

the basic binomial (Pascal triangle) identity.

12.5: For lumpability, check that for every pair of sets  $E_\xi$  and  $E_\eta$ ,  $\sum_{x_\nu \in E_\eta} p_{i\nu}$  has the same value for every  $x_i \in E_\xi$ . These common values form the transition probabilities  $\hat{p}_{\xi,\eta}$  for the lumped chain. If  $\xi$  and  $\eta$  differ by more than 1, then for every  $x_i \in E_\xi$ ,  $p_{i,\nu} = 0$  for  $\nu \in E_\eta$ , so  $\sum_{x_\nu \in E_\eta} p_{i\nu} = 0$ . If  $\xi - \eta = 1$  then for every  $x_i \in E_\xi$ ,  $p_{i,\nu} = \frac{1}{n}$  and  $\sum_{x_\nu \in E_\eta} p_{i\nu} = \frac{\xi}{n}$ . If  $\xi - \eta = -1$  then for every  $x_i \in E_\xi$ ,  $p_{i,\nu} = \frac{1}{n}$  and  $\sum_{x_\nu \in E_\eta} p_{i\nu} = \frac{n-\xi}{n}$ . This proves the lumpability criterion.

12.6:

$$P = \begin{matrix} & \begin{matrix} 000 & 100 & 010 & 001 & 101 & 011 & 110 & 111 \end{matrix} \\ \begin{matrix} 000 \\ 100 \\ 010 \\ 001 \\ 101 \\ 011 \\ 110 \\ 111 \end{matrix} & \begin{pmatrix} 1/2 & 1/6 & 1/6 & 1/6 & 0 & 0 & 0 & 0 \\ 1/6 & 1/2 & 0 & 0 & 1/6 & 0 & 1/6 & 0 \\ 1/6 & 0 & 1/2 & 0 & 0 & 1/6 & 1/6 & 0 \\ 1/6 & 0 & 0 & 1/2 & 1/6 & 1/6 & 0 & 0 \\ 0 & 1/6 & 0 & 1/6 & 1/2 & 0 & 0 & 1/6 \\ 0 & 0 & 1/6 & 1/6 & 0 & 1/2 & 0 & 1/6 \\ 0 & 1/6 & 1/6 & 0 & 0 & 0 & 1/2 & 1/6 \\ 0 & 0 & 0 & 0 & 1/6 & 1/6 & 1/6 & 1/2 \end{pmatrix} \end{matrix}.$$

The transition probability matrix is symmetric so the random walk Markov chain is reversible with stationary vector previously determined to be

$$\boldsymbol{\pi} = (1/8, 1/8, 1/8, 1/8, 1/8, 1/8, 1/8, 1/8).$$

The eigenvalues of  $P$  are  $1, 2/3, 1/3, 0$  with multiplicities  $1, 3, 3, 1$  respectively, so  $\lambda_2 = 2/3$ .

The partition is

$$\hat{S} = \{E_0, E_1, E_2, E_3\} = \{\{000\}, \{100, 010, 001\}, \{101, 011, 110\}, \{111\}\}.$$

The lumped transition probability matrix is

$$\hat{P} = \begin{matrix} & \begin{matrix} E_0 & E_1 & E_2 & E_3 \end{matrix} \\ \begin{matrix} E_0 \\ E_1 \\ E_2 \\ E_3 \end{matrix} & \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/6 & 1/2 & 2/6 & 0 \\ 0 & 2/6 & 1/2 & 1/6 \\ 0 & 0 & 1/2 & 1/2 \end{pmatrix} \end{matrix}$$

with  $\hat{\pi} = (1/8, 3/8, 3/8, 1/8)$ .

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$V = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$VUP = \begin{pmatrix} 1/2 & 1/6 & 1/6 & 1/6 & 0 & 0 & 0 & 0 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/9 & 1/9 & 1/9 & 0 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/9 & 1/9 & 1/9 & 0 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/9 & 1/9 & 1/9 & 0 \\ 0 & 1/9 & 1/9 & 1/9 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0 & 1/9 & 1/9 & 1/9 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0 & 1/9 & 1/9 & 1/9 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0 & 0 & 0 & 0 & 1/6 & 1/6 & 1/6 & 1/2 \end{pmatrix}.$$

Because the stationary distribution is uniform, the  $\pi$ -norm is simply scaling the standard Euclidean norm by  $\sqrt{8}$ . Then use the following R script.

```

1      # Enter matrices by rows, so use keyword byrow
2      P <- matrix( c(1/2,
3                    1/6, 1/6, 1/6, 0, 0, 0, 0, 1/6, 1/2, 0, 0, 1/
4                    6, 0, 1/6, 0, 1/6,
5                    0, 1/2, 0, 0, 1/6, 1/6, 0, 1/6, 0, 0, 1/2, 1/
6                    6, 1/6, 0, 0, 0,
7                    1/6, 0, 1/6, 1/2, 0, 0, 1/6, 0, 0, 1/6, 1/6,
8                    0, 1/2, 0, 1/6, 0,
9                    1/6, 1/6, 0, 0, 0, 1/2, 1/6, 0, 0, 0, 0, 1/6,
10                   1/6, 1/6, 1/2),
11                byrow=TRUE, nrow=8, ncol=8)
12
13     V <- matrix( c(1, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0,
14                   0, 0, 1, 0, 0,
15                   0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0,
16                   1), byrow=TRUE,
17                 nrow=8, ncol=4)
18
19     U <- matrix( c(1, 0, 0, 0, 0, 0, 0, 0, 0, 1/3,
20                   1/3, 1/3, 0, 0,
```

```

14      0, 0, 0, 0, 0, 0, 1/3, 1/3, 1/3, 0, 0, 0, 0,
      0, 0, 0, 0, 1),
15      byrow=TRUE, nrow=4, ncol=8)
16
17      D <- diag(1/sqrt(8), nrow=8, ncol=8)
18      Dinverse <- diag(sqrt(8), nrow=8, ncol=8)
19
20      lambda2 <- 2/3
21
22      N <- 10
23      H <- V %*% U %*% P
24      Hn <- H
25      Pn <- P
26
27      normdifference <- c( norm( Dinverse %*% (Hn - Pn)
      %*% D, type="2") )
28      for (n in 1:(N-1)) {
29          Hn <- H %*% Hn
30          Pn <- P %*% Pn
31          normdifference <- c( normdifference, norm(
      Dinverse %*% (Hn - Pn) %*% D, type="2") )
32      }
33      plot(normdifference, col="blue")
34
35      K <- function(n, l2) { n * l2^{n-1} }
36      points(K(1:N, lambda2), col="red")
37

```

12.7: (1) For the lumped chain,

$$\|pV\|_{\hat{\pi}} = \sqrt{(1/12)^2/(1/5) + (11/12)^2/(4/5)} = \sqrt{625/576} \approx 1.042.$$

For the original chain

$$\|p\|_{\pi} = \sqrt{(1/6)^2/(2/5) + (1/12)^2/(1/5) + (3/4)^2/(2/5)} = \sqrt{145/96} \approx 1.229.$$

(2) The definitions of the respective norms are

$$\|pV\|_{\hat{\pi}} = \sqrt{\sum_{\nu} (pV)_{\nu}^2 / \hat{\pi}_{\nu}}.$$

and

$$\|p\|_{\pi} = \sqrt{\sum_{\nu} p_{\nu}^2 / \pi_{\nu}}$$

It suffices to show that for any  $E_{\xi}$  in the partition

$$\sum_{\nu \in E_{\xi}} (p_{\nu})^2 / \pi_{\xi} \leq \sum_{\nu \in E_{\xi}} p_{\nu}^2 / \pi_{\nu}.$$

At first glance, this appears to be an application of a variant of the Cauchy-Schwarz Inequality or Jensen's Inequality. However, the inequality is not in the right form for either.

First take the case with 2 components  $x_1$  and  $x_2$  in  $E_\xi$  and consider the expression in the form

$$\frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} - \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} = \frac{\pi_2 x_1^2 - 2\pi_1 \pi_2 x_1 x_2 + \pi_1 x_2^2}{\pi_1 \pi_2 (\pi_1 + \pi_2)} = \frac{(\pi_2 x_1 - \pi_1 x_2)^2}{\pi_1 \pi_2 (\pi_1 + \pi_2)} \geq 0$$

so the expression is positive semi-definite, as expected. Note that the expression is 0 along the line  $(\pi_1 t, \pi_2 t)$ .

Next take the case with 3 components  $x_1, x_2$  and  $x_3$  in  $E_\xi$ .

$$\begin{aligned} \frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} + \frac{x_3^2}{\pi_3} - \frac{(x_1 + x_2 + x_3)^2}{\pi_1 + \pi_2 + \pi_3} = \\ \frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} - \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} + \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} + \frac{x_3^2}{\pi_3} - \frac{(x_1 + x_2 + x_3)^2}{\pi_1 + \pi_2 + \pi_3}. \end{aligned}$$

The two-component expression

$$\frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} - \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2}$$

is nonnegative as shown above. Then consider

$$\frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} + \frac{x_3^2}{\pi_3} - \frac{(x_1 + x_2 + x_3)^2}{\pi_1 + \pi_2 + \pi_3}.$$

as a similar two-component solution say with  $u_1 = (x_1 + x_2)$ ,  $u_2 = x_3$ ,  $\rho_1 = (\pi_1 + \pi_2)$  and  $\rho_2 = \pi_3$ . Then it too will be nonnegative, and the original three-component expression will be positive semidefinite. Note that the three-component expression is 0 along the line  $(\pi_1 t, \pi_2 t, \pi_3 t)$ .

Continue this process inductively until the entire original expression is shown to be nonnegative and the inequality holds.

12.8:

$$\begin{aligned} \|x_0 V \hat{P}^n - x_0 P^n V\|_{\hat{\pi}} &= \|x_0 V U P^n V - x_0 P^n V\|_{\hat{\pi}} \\ &= \|(x_0 V U P^n - x_0 P^n) V\|_{\hat{\pi}} \\ &\leq \|(x_0 V U P^n - x_0 P^n)\|_{\pi} \\ &\leq \|x_0\| \cdot \|V U P^n - P^n\|_{\pi} \\ &\leq \|x_0\| \cdot K(n) \cdot \delta \leq \|x_0\| \cdot n \cdot |\lambda_2|^{n-1} \cdot \delta. \end{aligned}$$

1: If  $\sigma = [123]$  and the transposition is  $(1, 2)$ , then  $\sigma^* = (1, 2)[123] = [213]$ , with  $d(\sigma^*, \sigma_0) = 1$  while  $d(\sigma, \sigma_0) = 0$ . The second case applies and the transition probability  $P([123], [213]) = \theta/3$ . Similar calculations apply for  $(1, 3)$  with  $\sigma^* = [321]$  and  $(2, 3)$  with  $\sigma^* = [132]$ . This is enough information to fill the first row of the transition probability matrix.

If  $\sigma = [132]$  and the transposition is  $(1, 2)$ , then  $\sigma^* = (1, 2)[132] = [231]$ , with  $d(\sigma^*, \sigma_0) = 2$  while  $d(\sigma, \sigma_0) = 1$ . The second case applies and the transition probability  $P([132], [231]) = \theta/3$ . If  $\sigma = [132]$  and the transposition is  $(1, 3)$ , then  $\sigma^* = (1, 3)[132] = [312]$ , with  $d(\sigma^*, \sigma_0) = 2$  while  $d(\sigma, \sigma_0) = 1$ . The second case applies again and the transition probability  $P([132], [312]) = \theta/3$ .

If  $\sigma = [132]$  and the transposition is  $(2, 3)$ , then  $\sigma^* = (2, 3)[132] = [123]$ , with  $d(\sigma^*, \sigma_0) = 0$  while  $d(\sigma, \sigma_0) = 1$ . The first case applies again and the transition probability  $P([132], [123]) = 1/3$ . Similar calculations apply for  $(1, 3)$  with  $\sigma^* = [312]$  and  $(2, 3)$  with  $\sigma^* = [132]$ . This enough information to complete the fourth row of the transition probability matrix.

If  $\sigma = [312]$  and the transposition is  $(1, 2)$ , then  $\sigma^* = (1, 2)[312] = [321]$ , with  $d(\sigma^*, \sigma_0) = 1$  while  $d(\sigma, \sigma_0) = 2$ . The first case applies and the transition probability  $P([312], [321]) = 1/3$ . Similar calculations apply for  $(1, 3)$  with  $\sigma^* = [132]$  and  $(2, 3)$  with  $\sigma^* = [213]$ .

The other rows are similar.

2: For  $\theta = 1/2$ ,  $P^{10}$  is (to three decimal places)

$$\begin{pmatrix} 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.334 & 0.166 & 0.166 & 0.166 & 0.084 & 0.084 \\ 0.334 & 0.166 & 0.166 & 0.166 & 0.084 & 0.084 \end{pmatrix}$$

agreeing with the stationary distribution.

3: The algorithm needs to shuffle an array in a way such that all  $n!$  permutations are equally likely. One important property of the  $n!$  permutations is that any given position (say  $j$ ) will be populated by a given element (say  $i$ ) with probability  $1/n$ . This is because, out of the  $n!$  permutations,  $(n-1)!$  contain element  $j$  at location  $i$ . Due to this equidistribution, we can try to first fix the element at a particular (in this case, the last) location and then process the remaining elements. The first step of the algorithm guarantees the probability of the last entry being  $j$  is  $1/n$ , the second step of the algorithm guarantees the probability of the second-last entry being  $j$  is  $1/(n-1)$  and so on. Inductively then, the probability of a given permutation is  $1/n!$ .

1: Case 1: Suppose  $x'$  is chosen according to  $P(x, x')$  with  $x \neq x'$  and

$$A(x, x') = \frac{\pi(x')P(x', x)}{\pi(x)P(x, x')} \geq 1.$$

Then  $Q(x, x') = P(x, x')$  so the left side becomes  $\pi(x)Q(x, x') = \pi P(x, x')$ . On the right hand side, since  $A(x, x') \geq 1$ , then

$$A(x', x) = \frac{\pi(x)P(x, x')}{\pi(x')P(x', x)} \leq 1.$$

so

$$Q(x', x) = P(x', x)A(x', x) = P(x', x) \frac{\pi(x)P(x, x')}{\pi(x')P(x', x)}.$$

so  $\pi(x)Q(x', x) = \pi(x)P(x, x')$ .

Case 2: Case 1: Suppose  $x'$  is chosen according to  $P(x, x')$  with  $x \neq x'$  and

$$A(x, x') = \frac{\pi(x')P(x', x)}{\pi(x)P(x, x')} < 1.$$

is similar.

- 2: (a) For  $N = 3$ , the transition probability matrix is

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/9 & 4/9 & 4/9 & 0 \\ 0 & 4/9 & 4/9 & 1/9 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

- (b) The stationary distribution is  $\pi = (1/20, 9/20, 9/20, 1/20)$ .  
 (c) For simplicity and without prior knowledge on the transitions among the 4 states choose

$$\begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{pmatrix}.$$

Then the denominator of the  $\alpha_{ij}$  values is

$$\alpha_{ij} = \frac{1}{1 + \frac{\pi_i p_{ij}}{\pi_j p_{ji}}} = \frac{1}{1 + \frac{\pi_i}{\pi_j}}.$$

The matrix of  $\alpha_{ij}$  values is

$$\begin{pmatrix} \frac{1}{2} & \frac{9}{10} & \frac{9}{10} & \frac{1}{2} \\ \frac{1}{10} & \frac{1}{2} & \frac{1}{2} & \frac{1}{10} \\ \frac{1}{10} & \frac{9}{10} & \frac{9}{10} & \frac{1}{10} \\ \frac{1}{2} & \frac{1}{10} & \frac{1}{10} & \frac{1}{2} \end{pmatrix}.$$

Since all entries are between 0 and 1, choose  $s_{ij} = 1$ . Then the matrix  $Q$  for the Metropolis-Hastings algorithm is

$$\begin{pmatrix} \frac{17}{40} & \frac{9}{40} & \frac{9}{40} & \frac{1}{8} \\ \frac{1}{40} & \frac{33}{40} & \frac{1}{40} & \frac{1}{40} \\ \frac{1}{40} & \frac{1}{40} & \frac{33}{40} & \frac{1}{40} \\ \frac{1}{8} & \frac{9}{40} & \frac{9}{40} & \frac{17}{40} \end{pmatrix}.$$

This has the same stationary distribution.

- (d) The eigenvalues of  $P$  are  $1, 1/3, -1/9, -1/3$ . The rate of convergence to the stationary distribution is approximately  $(1/3)^n$ .  
 (e) The eigenvalues of  $Q$  are  $1, 7/10, 1/2, 3/10$ . The rate of convergence to the stationary distribution is approximately  $(7/10)^n$ , much slower.
- 3: (a) Since each state has a positive probability of transitioning to its neighbor state, the chain is irreducible. Alternatively, each entry in  $P^4$  is non-zero, so the chain is irreducible. Since this is a finite state space irreducible chain, it is positive recurrent. Since each state has a positive probability of staying in the state, the minimum return time is 1, so the chain is aperiodic.
- (b)

$$\pi = \left( \frac{1}{16}, \frac{1}{4}, \frac{3}{8}, \frac{1}{4}, \frac{1}{16} \right).$$

- (c) It is easy to check the reversibility, but both the physical description, and the symmetry of  $\pi$  and  $P$  suggest that reversibility holds.  
 (d) The eigenvalues, ordered by decreasing value, are  $1, 3/4, 1/2, 1/4, 0$ .



(e) The corresponding eigenvectors, without normalization, are

$$(1, 1, 1, 1, 1)^T, (1, 1/2, 0, -1/2, -1)^T, (1, 0, -1/3, 0, 1)^T, \\ (1, -1/2, 0, 1/2, -1)^T, (1, -1, 1, -1, 1)^T.$$

(f) The weighted inner products of each eigenvector with itself is respectively  $1, 1/4, 1/6, 1/4, 1$  so the normalized eigenvectors are

$$(1, 1, 1, 1, 1)^T, (2, 1, 0, -1, -2)^T, \left( \sqrt{6}, 0, -\frac{\sqrt{6}}{3}, 0, \sqrt{6} \right)^T, \\ (2, -1, 0, 1, -2)^T, (1, -1, 1, -1, 1)^T.$$

(g) With (for example) the Maxima command

```
generateP: genmatrix(lambda([i,j], pi[j] *
sum(lambda[k]*psi[k][i]*psi[k][j], k, 1, 5)[1]), 5, 5);
the result is
```

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{8} & \frac{1}{2} & \frac{3}{8} & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\ 0 & 0 & \frac{3}{8} & \frac{1}{2} & \frac{1}{8} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

as expected.

- 4: (a) Using the normalized eigenvectors from the previous solution, the upper bound is:

$$\frac{1}{4} \sum_{i=2}^{\text{card}(\mathcal{X})} \lambda_i^{2n} \psi_i(x)^2 \\ = \frac{1}{4} \left[ \left( \frac{3}{4} \right)^{2n} \cdot (-2)^2 + \left( \frac{1}{2} \right)^{2n} \cdot (\sqrt{6})^2 + \left( \frac{1}{4} \right)^{2n} \cdot (-2)^2 + (0)^{2n} (-2)^2 \right] \\ = \left( \frac{3}{4} \right)^{2n} + \frac{3}{2} \cdot \left( \frac{1}{2} \right)^{2n} + \left( \frac{1}{4} \right)^{2n}$$

- (b) After 5 steps, the total variation distance squared is approximately 0.0359 and the upper bound is approximately 0.0578 so the inequality bound holds. After 10 steps, the total variation distance squared is approximately 0.00181 and the upper bound is approximately 0.00317 so the inequality bound holds.

5:

$$\begin{aligned}
\langle Pg, h \rangle &= \sum_x \sum_y P(x, y) g(y) h(x) \pi(x) \\
&= \sum_x \sum_y g(y) h(x) \pi(x) P(x, y) \\
&= \sum_x \sum_y g(y) h(x) \pi(y) P(y, x) \\
&= \sum_x \sum_y g(y) P(y, x) h(x) \pi(y) \\
&= \sum_y \sum_x g(y) P(y, x) h(x) \pi(y) \\
&= \sum_y g(y) \sum_x P(y, x) h(x) \pi(y) \\
&= \langle g, Ph \rangle.
\end{aligned}$$

6: Let  $\mathbf{e}_x$  be the elementary column vector with 1 at position  $x$  and 0 elsewhere.

Since  $\mathbf{e}_x$  is a probability distribution concentrated entirely on state  $x$ , then  $\mathbf{e}_x^T \cdot P$  is the probability distribution of states after one step from  $x$ . Then  $\mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y$  picks out  $P(x, y)$ , that is,  $\mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y = P(x, y)$ . The point is that this probability product does not involve the inner product weight vector  $\pi$ .

The orthonormal eigenvector basis represents  $\mathbf{e}_x$  in terms of  $\psi_i$  as  $\mathbf{e}_x = \sum_i a_{xi} \psi_i$  for some scalars  $a_{xi}$ . Projecting  $\mathbf{e}_x$  against  $\psi_i$  with the weighted inner product

$$a_{xi} = \langle \mathbf{e}_x, \psi_i \rangle = \psi_i(x) \pi(x)$$

so as a column vector

$$\mathbf{e}_x = \sum_i \psi_i(x) \pi(x) \psi_i.$$

Using

$$P(x, y) = \mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y$$

where  $\mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y$  indicates the usual matrix-vector product with rows dotted against columns, and expressing  $\mathbf{e}_y$ , but not  $\mathbf{e}_x$ , in terms of the orthonormal basis

$$\begin{aligned}
&= \mathbf{e}_x \cdot P \cdot \left( \sum_i \psi_i(y) \pi(y) \psi_i \right) \\
&= \mathbf{e}_x \cdot \left( \sum_i \psi_i(y) \pi(y) P \cdot \psi_i \right) \\
&= \mathbf{e}_x \cdot \left( \sum_i \psi_i(y) \pi(y) \lambda_i \psi_i \right)
\end{aligned}$$

using the eigenvector property. Now factoring the dot product with  $\mathbf{e}_x$  through the sum will pick out the  $x$ th term from each  $\psi_i$ ,

$$\begin{aligned} &= \sum_i \psi_i(y) \pi(y) \lambda_i (\mathbf{e}_x \cdot \psi_i) \\ &= \sum_i \psi_i(y) \pi(y) \lambda_i \psi_i(x) \end{aligned}$$

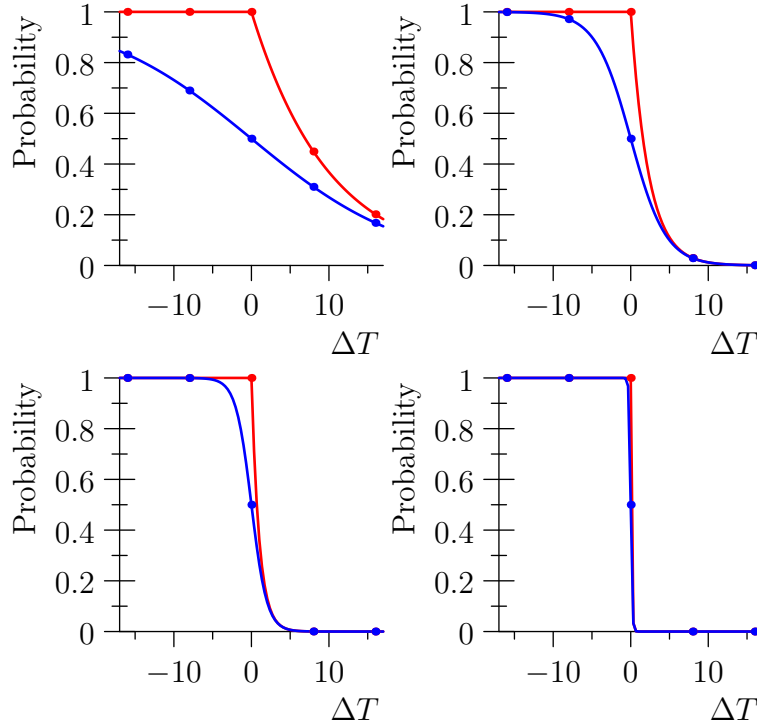
and finally,  $\pi(y)$  is independent of the summation over  $i$  so it can be factored out of the sum, and rearranging the products yields

$$= \pi(y) \sum_i \lambda_i \psi_i(x) \psi_i(y).$$

- 1: With  $n$  sites, the chance of missing a site is  $1 - \frac{1}{n}$ . In  $n$  iterations of the selection, the chance of missing the site is  $(1 - \frac{1}{n})^n \approx 1/e$  for  $n$  large. Among  $n$  sites there will be approximately  $1/e \cdot n$  sites missed.
- 2:

$$\Delta E = E(\omega') - E(\omega) = -2J(\omega'_{(i,j)} - \omega_{(i,j)}) \sum_{k=1}^4 \omega_{\langle i,j \rangle[k]}$$

where the sum is only over the four nearest neighbors of the  $(i, j)$  site. The difference  $(\omega'_{(i,j)} - \omega_{(i,j)}) = \pm 2$ . The sum over the four nearest neighbors will be  $\pm 4$  if all 4 neighbors have the same sign,  $\pm 2$  if 3 neighbors have the same sign, and 0 if 2 are opposite, and 0 if 2 of the neighbors have one sign, and the other 2 are opposite. Then  $\Delta E$  can only have the values  $-16, -8, 0, +8, +16$ .



3:

4: For the Metropolis chains with the deterministic visitation rule, consider configuration  $\omega$  and configuration  $\omega'$  which differs in one site. It is possible to go from  $\omega$  to  $\omega'$  in at most  $N^2$  steps, each of which has non-zero probability (although it may be small!) of occurring. That is, all configurations communicate, and the chain is irreducible.

The same argument holds for the Glauber chain with the random selection visitation rule, although the expected time to reach one state from another is longer as in the coupon collectors problem, and the probability of movement is smaller.

5: An important feature of the puzzle is that all fleas move independently. The problem has two challenges:

- not all squares on a grid are created equal since edge squares have fewer neighbors than interior squares, and
- the process lasts for only 50 periods, so without further investigation, it is not apparent how close it is to a stationary distribution.

The last item means that the solution will have to be computational.

To build an intuition, assume instead all squares are equal and that 50 can be considered a long period of time. Then a flea can be in one of the  $30 \cdot 30 / 2 = 450$  squares with equal probability. Why 450 and not 900? To see this assume the grid was painted in black and white like a chessboard. After 50 moves a flea starting on a white square must be on a white square; similarly a flea starting on a black square must be on a black square. This is similar to the reasoning in 1-dimensional random walk that after an even number of steps, the walker is at an even-numbered position.

What is the probability that some given square is empty after 50 moves? There are 450 fleas that potentially independently can occupy it. (Notice that any flea can reach any square in no more than 60 jumps.) Therefore the probability that a square is *not* occupied by any flea is  $(1 - 1/450)^{450} \approx e^{-1} \approx 0.367470$ . Taking expectations over all 900 fleas, the number of empty squares will be  $900 \cdot (1 - 1/450)^{450} \approx 330.723$ .

However, the variance will be approximately  $e^{-1}(1 - e^{-1})/N \approx \frac{0.23254}{N}$ . To get the answer to six decimal places means the estimate will need to have at least  $\sqrt{\frac{0.23254}{N}} < 5 \times 10^{-7}$ , or at least  $N > 9.3 \times 10^{11}$  or more than  $900 \cdot 9.3 \times 10^{11} = 8.4 \times 10^{14}$  flea moves. Even with current modern processors working in parallel, simulation will take too long to achieve the desired accuracy.

Making 10,000 simulations of 50 steps each using the following script gives a mean value of 331.8646.

```

1 # set.seed(2023)                                #for testing,
   debugging
2 N <- 30
3 sims <- 10000
4
5 inbounds <- function(x) { all(x >= 1) && all(x <= N)
   }

```

```

6
7 # Denote the location of a flea by (i, j). Here is a
  function
8 # that gives us a _list_ of locations where a flea at
  (i,j) can jump.
9 # The key element of this function is removing
  potential locations that
10 # are out of bounds.
11 neighbors <- function(site) {
12   adjacencies <- list( c(1,0), c(-1,0), c(0, 1), c
     (0,-1) )
13   nbrs <- lapply(adjacencies, function(x) x + site)
14   realNbrs <- sapply(nbrs, inbounds)
15   nbrs[ realNbrs ]
16 }
17
18 # Create two helper
19 # functions that recode (i, j) position of a flea to
  its numeric index:
20 site2i <- function(site) {
21   site[1] + (site[2] - 1) * N
22 }
23
24 i2site <- function(i) {
25   s <- c( ( (i-1) %% N + 1 ), ((i-1) %/% N + 1) )
26   return(s)
27 }
28
29 # Create a list, which in cell (i, j) recoded by
  site2i( (i,j) )
30 # stores the target locations for a flea:
31 NEI <- list()
32 for (i in 1:N) {
33   for (j in 1:N) {
34     s <- site2i( c(i,j) )
35     NEI[[s]] <- neighbors( c(i,j) )
36   }
37 }
38
39 # The idea of the simulation is to initialize it
  with N^2 fleas,
40 # each starting on a different square, recoded by
  site2i
41 fleas <- list()
42 for (i in 1:N) {
43   for (j in 1:N) {
44     s <- site2i( c(i,j) )

```

```

45     fleas[[s]] <- c(i,j)
46   }
47 }
48
49 result <- numeric(sims)
50
51 for (sim in 1:sims) {
52   # Then each flea on a square moves randomly to one of
53   # the locations it is allowed to occupy.
54   for (i in 1:N^2) {
55     f <- fleas[[i]]           #find
56     site flea is on now
57     s <- site2i(f)           #recode
58     to position in NEI
59     l <- length(NEI[[s]] )   #count
60     adjacent sites
61     r <- sample(1:l, 1)      #choose
62     one randomly
63     newSite <- NEI[[s]][[r]]  #fix
64     newSite as the chosen
65     fleas[[i]] <- newSite     #make
66     that new site for flea i
67   }
68
69   # Create a matrix to record unoccuied squares.
70   # Initially it will say all sites are unoccupied
71   # (with a 1 for TRUE).
72   unoccupied <- matrix(1, N, N)
73   # If a site is occupied after a jump, change to 0
74   # (FALSE).
75   for (i in 1:N^2) {
76     unoccupied[ i2site(fleas[[i]])[1], i2site(
77     fleas[[i]])[2] ] <- 0
78   }
79   result[sim] <- sum(unoccupied)
80 }
81
82 mean(result)

```

Using the following script, using floating point calculation and the Markov chain nature of the problem, the probability to 6 figures is 330.721. (The script is a naive implementation without consideration for efficiency. It still runs quickly.)

```

1 library(expm)
2 N <- 30

```

```

3
4 surroundNeighbors <- function(site) {
5   belowSite <- if (site[1] == N) NULL else c(site
6     [1]+1, site[2])
7   leftSite <- if (site[2] == 1) NULL else c(site
8     [1], site[2]-1)
9   aboveSite <- if (site[1] == 1) NULL else c(site
10    [1]-1, site[2])
11   rightSite <- if (site[2] == N) NULL else c(site
12    [1], site[2]+1)
13   neighbors <- rbind(belowSite, leftSite,
14     aboveSite, rightSite)
15 }
16
17 site2i <- function(site) {
18   site[1] + (site[2] - 1) * N
19 }
20
21 i2site <- function(i) {
22   c( ( (i-1) %% N + 1 ), ((i-1) %/% N + 1) )
23 }
24
25 T = matrix(0, N^2, N^2)
26
27 for (i in 1:N^2) {
28   nbrs <- surroundNeighbors( i2site(i) )
29   for (k in 1:nrow(nbrs)) {
30     nbr <- nbrs[k, ]
31     T[i, site2i(nbr)] <- 1/nrow(nbrs)
32   }
33 }
34
35 complementT50 <- 1 - T %>% 50
36 emptyCells <- sum(apply(complementT50, 2, prod))
37 emptyCells

```

The following Julia scripts are efficient implementations of the simulation and theoretical analyses.

```

1 const N = 30
2
3 neighbors(c::Tuple{Int, Int}) =
4   filter!([c .+ d for d in ((1, 0), (-1, 0), (0, 1),
5     (0, -1))]) do new_c
6     all(x -> 1 <= x <= N, new_c)
7   end

```

```

7  # The key element of this function is removing new
   # potential locations that
8  # are out of bounds.
9
10 const NEI = [neighbors((i, j)) for i in 1:N, j in 1:N
   ]
11
12 function sim(steps)
13     fleas = [(i, j) for i in 1:N, j in 1:N]
14     for _ in 1:steps
15         for i in eachindex(fleas)
16             fleas[i] = rand(NEI[fleas[i]...])
17             # note the splatting, expanding to
multiple positional args
18         end
19     end
20     unoccupied = trues(N, N)
21     for c in fleas
22         unoccupied[c...] = false
23     end
24     return sum(unoccupied)
25 end
26 # The idea of the simulation is to initialize it with
   # 900 fleas, each
27 # starting on a different square. Then each of them
   # moves randomly to one of
28 # the locations it is allowed to occupy. Finally,
   # count the number of
29 # unoccupied squares.
30
31 using Statistics
32 using Random
33 Random.seed!(1234);
34
35 simres = [sim(50) for _ in 1:10_000]
36 mean(simres)
37 # Additionally compute the 90% confidence interval
   # for the estimator using bootstrapping:
38 quantile([mean(rand(simres, length(simres))) for _ in
   1:10_000],
39           [0.05, 0.95])

```

```

1  const N = 30
2
3  neighbors(c::Tuple{Int, Int}) =

```



```

4      filter!([c .+ d for d in ((1, 0), (-1, 0), (0, 1)
      , (0, -1))]) do new_c
5          all(x -> 1 <= x <= N, new_c)
6      end
7  # The key element of this function is removing new
      potential locations that
8  # are out of bounds.
9
10 const NEI = [neighbors((i, j)) for i in 1:30, j in 1:
      N]
11
12 # build a transition
13 # probability matrix for the problem. For this, first
      create two helper
14 # functions that recode (i, j) position of a flea to
      its numeric index:
15 c2i(c::Tuple{Int, Int}) = c[1] + (c[2] - 1) * N
16 i2c(i::Int) = reverse(divrem(i - 1, N)) .+ (1, 1)
17
18 # The location TRANS[i, j] encodes the probability
      that flea starting from
19 # location i (encoded using linear index) ends up in
      location j. Therefore
20 # the sum of probabilities in rows are all equal to
      one.
21 const TRANS = zeros(N^2, N^2)
22 for i in 1:N^2
23     ni = c2i.(neighbors(i2c(i)))
24     TRANS[i, ni] .= 1 / length(ni)
25 end
26
27 # the TRANS ^ 50 matrix encodes probability that flea
      starting from
28 # location i ends up in location j after 50 moves. 1
      .- TRANS ^ 50 is
29 # a matrix, where TRANS[i, j] is the probability that
      flea
30 # starting in position i is not in position j after
      50 moves. Since
31 # fleas move independently prod(1 .- TRANS^50, dims
      =1) gives a
32 # probability for each cell that it is not occupied
      by any flea. Using
33 # linearity of expectation again, the expected number
      of
34 # unoccupied cells is sum(prod(1 .- TRANS^50, dims=1)
      ).

```

```

35 |
36 | round(sum(prod(1 .- TRANS^50, dims=1)), digits=6)

```

**Remark 21.18.** This problem is slightly adapted from the Project Euler Problem 213. The solution and the Julia scripts are adapted from Flea circus for the New Year celebration. A detailed discussion of the simulation approach is at How should one approach Project Euler problem 213?. Another solution using multinomial distributions is at R-bloggers: Flea Circus

1: The algebra is tedious but routine. Checking just the first entry is representative. The first-row, first-column entry of  $P_{X|X}$  is

$$\frac{p_1^2}{(p_1 + p_3)(p_1 + p_2)} + \frac{p_3^2}{(p_1 + p_3)(p_3 + p_4)}$$

and the second-row, first-column entry of  $P_{X|X}$  is

$$\frac{p_1 p_2}{(p_2 + p_4)(p_3 + p_4)} + \frac{p_3 p_4}{(p_2 + p_4)(p_3 + p_4)}.$$

The dot product of the row-vector  $f = (p_1 + p_3, p_2 + p_4)$  with the elements making this column gives

$$\frac{p_1^2}{(p_1 + p_2)} + \frac{p_3^2}{(p_3 + p_4)} + \frac{p_1 p_2}{(p_1 + p_2)} + \frac{p_3 p_4}{(p_3 + p_4)}.$$

The sum of the first and third fractions simplifies to  $p_1$ , the sum of the second and fourth fractions simplifies to  $p_3$  and the total is  $p_1 + p_3$ .

2:

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x, y) \, dy &= \int_{-\infty}^{\infty} \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)}} \, dy \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{\rho^2 x^2-2\rho xy+y^2}{2(1-\rho^2)}} \, dy \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{(\rho x-y)^2}{2(1-\rho^2)}} \, dy \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{z^2}{2(1-\rho^2)}} \, dz \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{u^2}{2}} \sqrt{1-\rho^2} \, du \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \sqrt{2\pi(1-\rho^2)} \\
&= \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}.
\end{aligned}$$

3:

$$\begin{aligned}
f_{x|y}(x|y) &= f(x, y)/f_y(y) \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)}} / \frac{1}{\sqrt{2\pi}} e^{-y^2/2} \\
&= \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)} + \frac{(1-\rho^2)y^2}{2(1-\rho^2)}} \\
&= \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{x^2-2\rho xy+\rho^2 y^2}{2(1-\rho^2)}} \\
&= \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{(x-\rho y)^2}{2(1-\rho^2)}}.
\end{aligned}$$

1:

$$\begin{aligned}
\int_0^\infty \frac{e^{-\theta} \theta^x}{x!} e^{-\theta} d\theta &= \frac{1}{x!} \int_0^\infty e^{-2\theta} \theta^x d\theta \\
&= \frac{1}{x!} \cdot \frac{1}{2^{x+1}} \int_0^\infty e^{-2\theta} (2\theta)^x d(2\theta) \\
&= \frac{1}{x!} \cdot \frac{1}{2^{x+1}} \cdot x!
\end{aligned}$$

where the last equality is the factorial property of the Gamma integral.

2:

$$\begin{aligned}
\int_0^\infty \frac{2^{x+1} \theta^{x+x'} e^{-3\theta}}{x!x'!} d\theta &= \frac{2^{x+1}}{x!x'!} \int_0^\infty \theta^{x+x'} e^{-3\theta} d\theta \\
&= \frac{2^{x+1}}{3^{x+x'+1} x!x'!} \int_0^\infty (3\theta)^{x+x'} e^{-3\theta} d(3\theta) = \frac{2^{x+1}}{3^{x+x'+1} x!x'!} (x+x')! \\
&= \frac{2^{x+1}}{3^{x+x'+1}} \binom{x+x'}{x}.
\end{aligned}$$

3:

$$\begin{aligned}
&\left(\frac{1}{1+\alpha}\right)^a \sum_{x=0}^\infty \frac{(a)_x}{x!} \left(\frac{\alpha}{\alpha+1}\right)^x \\
&= \left(\frac{1}{1+\alpha}\right)^a \left[ 1 + \frac{a}{1!} \left(\frac{\alpha}{\alpha+1}\right) + \frac{a(a+1)}{2!} \left(\frac{\alpha}{\alpha+1}\right)^2 + \dots \right] \\
&= \left(\frac{1}{1+\alpha}\right)^a \left[ 1 - \frac{-a}{1!} \left(\frac{\alpha}{\alpha+1}\right) + \frac{-a(-a-1)}{2!} \left(\frac{\alpha}{\alpha+1}\right)^2 + \dots \right] \\
&= \left(\frac{1}{1+\alpha}\right)^a \left[ 1 - \frac{\alpha}{\alpha+1} \right]^{-a} = 1
\end{aligned}$$

where the next-to-last equality is from the general Binomial Expansion or equivalently the Taylor expansion of  $(1+z)^{-a}$ .

4: Move terms in the denominator not depending on  $\lambda$  out of the integral and combine like terms in the numerator.

$$\begin{aligned} k(x, y) &= \int_0^\infty \frac{e^{-\lambda(\alpha+1)/\alpha} \lambda^{a+x-1}}{\Gamma(a+x)(\alpha/(\alpha+1))^{a+x}} \cdot \frac{e^{-\lambda} \lambda^y}{y!} d\lambda \\ &= \frac{1}{\Gamma(a+x)(\alpha/(\alpha+1))^{a+x} y!} \int_0^\infty e^{-\lambda((\alpha+1)/\alpha+1)} \lambda^{a+x+y-1} d\lambda. \end{aligned}$$

Let  $z = \frac{2\alpha+1}{\alpha} \lambda$ , so  $d\lambda = \frac{\alpha}{2\alpha+1} dz$ . Then the integral becomes

$$\begin{aligned} &\int_0^\infty e^{-\lambda((\alpha+1)/\alpha+1)} \lambda^{a+x+y-1} d\lambda \\ &= \int_0^\infty e^{-z} z^{a+x+y-1} \left( \frac{\alpha}{2\alpha+1} \right)^{a+x+y} dz \\ &= \Gamma(a+x+y) \left( \frac{\alpha}{2\alpha+1} \right)^{a+x+y}. \end{aligned}$$

5: Use the definition of the Meixner polynomial

$$M_j(x; a, \alpha) = {}_2F_1(-j, -x; a; -\alpha)$$

in terms of the Gauss series for the regular hypergeometric function with  $a = -j$ ,  $b = -x$ ,  $c = a$  and  $z = -\alpha$ . For negative integer values of  $a$  the Gauss series terminates as a degree  $j$  polynomial. Then directly  $M_0(x) = 1$ , and  $M_1(x) = 1 + \frac{(-1)(-x)(-\alpha)}{1! \cdot a} = 1 - \frac{\alpha}{a}x$  and  $M_2(x) = 1 + \frac{(-1)(-x)(-\alpha)}{1! \cdot a} + \frac{(-2)(-1)(-x)(-x+1)\alpha^2}{2! \cdot a(a+1)} = 1 - \frac{\alpha(\alpha+a+1)}{a(a+1)}x + \frac{\alpha^2}{a(a+1)}x^2$ .

6: For  $j = k = 0$ ,

$$\sum_{x=0}^{\infty} M_0(x) M_0(x) m(x) = \sum_{x=0}^{\infty} m(x) = 1$$

because  $m(x)$ , the negative binomial distribution, is a probability distribution. This matches the given

$$\frac{(1+\alpha)^0 0!}{(a)_0} \delta_{00} = 1.$$

For  $j = 0$  and  $k = 1$

$$\begin{aligned} \sum_{x=0}^{\infty} M_0(x) M_1(x) m(x) &= \sum_{x=0}^{\infty} M_1(x) m(x) = \sum_{x=0}^{\infty} \left( 1 - \frac{\alpha}{a}x \right) m(x) \\ &= \sum_{x=0}^{\infty} m(x) - \frac{\alpha}{a} \sum_{x=0}^{\infty} x m(x) = 1 - \frac{\alpha}{a} \cdot a \cdot \frac{\alpha}{\alpha+1} \cdot \frac{1}{1/\alpha+1} = 1 - \frac{\alpha^2}{(\alpha+1)^2} \end{aligned}$$

by using the mean of the negative binomial distribution.

For  $j = k = 1$

$$\begin{aligned}
& \sum_{x=0}^{\infty} M_1(x) M_1(x) m(x) \\
&= \sum_{x=0}^{\infty} \left(1 - \frac{\alpha}{a} x\right)^2 m(x) \\
&= \sum_{x=0}^{\infty} m(x) - 2 \frac{\alpha}{a} \sum_{x=0}^{\infty} x m(x) + \frac{\alpha^2}{a^2} \sum_{x=0}^{\infty} x^2 m(x) \\
&= 1 - 2 \frac{\alpha}{a} \cdot a \cdot \frac{\alpha}{\alpha+1} \cdot \frac{1}{1/\alpha+1} + \frac{\alpha^2}{a^2} a \cdot \frac{\alpha}{\alpha+1} \cdot \frac{1}{(1/\alpha+1)^2} = 1 - 2\alpha^2 + \frac{\alpha^3(\alpha+1)}{\alpha}
\end{aligned}$$

by using the mean and variance of the negative binomial distribution.

7: Follow [Chi78, pages 4 and 176].

The generating function definition of the Meixner polynomials  $m_n(x, \beta, c)$  is

$$\left(1 - \frac{w}{c}\right)^x (1-w)^{-x-\beta} = \sum_{\nu=0}^{\infty} m_{\nu}(x; \beta, c) \frac{w^{\nu}}{n!}$$

The binomial expansion for the first factor in  $G(x, w)$  is  $\left(1 - \frac{w}{c}\right)^x$  is

$$\left(1 - \frac{w}{c}\right)^x = \sum_{\nu=0}^{\infty} (-1)^{\nu} \binom{x}{\nu} \frac{w^{\nu}}{c^{\nu}} = \sum_{\nu=0}^{\infty} \frac{(x)_n}{k!} \frac{w^{\nu}}{c^{\nu}}$$

where  $(x)_n$  is the falling Pochhammer symbol or falling factorial  $x(x-1)(x-2) \cdots (x-(n-1))$ .

The binomial expansion for the second factor in  $G(x, w)$  is

$$(1-w)^{-x-\beta} = \sum_{\nu=0}^{\infty} (-1)^{\nu} \binom{-x-\beta}{\nu} w^{\nu}.$$

Then multiplying the two expansions, collecting terms in powers of  $w$  gives for the coefficient  $n$

$$m_n(x, \beta, c) = (-1)^n n! \sum_{\nu=0}^n \binom{x}{\nu} \binom{-x-\beta}{n-\nu} c^{-\nu}.$$

The factor  $n!$  results from “multiply in  $n!$  and divide out  $n!$ ” to introduce the  $n!$  in denominator of the definition which was not originally present in the binomial expansions. The  $(-1)^n$  results from the  $(-1)^{\nu}$  from the first factor binomial expansion and the  $(-1)^{n-\nu}$  from the second factor binomial expansion. The  $c^{-\nu}$  comes from the denominator in the expansion of the first term.

Since  $\binom{x}{\nu} = \frac{1}{\nu!} x(x-1) \cdots (x-\nu+1)$  has degree  $\nu$  and  $\binom{-x-\beta}{n-\nu} = \frac{1}{(n-\nu)!} (-x-\beta)(-x-\beta-1) \cdots (-x-\beta-(n-\nu-1))$  has degree  $n-\nu$ ,  $m_n(x, \beta, c)$  is a polynomial of degree  $n$ .

Now an identity in the parameters of the Meixner polynomials

$$\begin{aligned}
 m_n(-x - \beta; \beta, c_{-1}) &= (-1)^n n! \sum_{\nu=0}^n \binom{-x - \beta}{\nu} \binom{-(x - \beta) - \beta}{n - \nu} (c^{-1})^{-\nu} \\
 &= (-1)^n n! \sum_{\nu=0}^n \binom{-x - \beta}{\nu} \binom{x}{n - \nu} c^\nu \\
 &= c^n (-1)^n n! \sum_{\nu=0}^n \binom{-x - \beta}{\nu} \binom{x}{n - \nu} c^{\nu - n} \\
 &= c^n (-1)^n n! \sum_{\nu_1=0}^n \binom{-x - \beta}{n - \nu_1} \binom{x}{\nu_1} c^{\nu_1} \\
 &= c^n m_n(x; \beta, c).
 \end{aligned}$$

- 1: Consider a representative node  $j$  with  $1 \leq j \leq n - 1$  with load  $q_j$  and neighboring node with load  $q_{j+1}$ . After one Markov chain step by  $P_{1/2}$  of load exchange the expected gain would be  $\frac{1}{2}q_{j+1} - \frac{1}{2}q_j$ . If  $q_{j+1} > q_j$ , the gain is positive, one-half of the load imbalance shifts from  $j + 1$  to  $j$ . If  $q_{j+1} < q_j$ , the gain is negative, one-half of the load imbalance shifts from  $j$  to  $j + 1$ . For the end node  $n$ , the calculation is similar.
- 2: The matrix  $(\mathbf{1}\mathbf{1}^T)$  has 1 in every entry. The matrix-vector product  $(\mathbf{1}\mathbf{1}^T) \mathbf{1}$  sums the rows, giving  $n\mathbf{1}$ , then  $(1/n) (\mathbf{1}\mathbf{1}^T) \mathbf{1} = \mathbf{1}$ .
- 3: There are two urns I and II containing a total of  $n$  balls. The state of the Markov chain is the number of balls in urn I so the number of states is  $n + 1$ . At each turn, with probability  $p$  a ball is taken from urn II and moved to urn I or with complementary probability  $q$  a ball is moved from urn I to urn II. If there are no balls in urn I then with probability  $q$  urn I stays empty. Similarly for the last state if urn I has all  $n$  balls.
- 4: Use the sum-to-product identity for cosines:

$$\cos(\theta) + \cos(\phi) = 2 \cos\left(\frac{\theta + \phi}{2}\right) \cdot \cos\left(\frac{\theta - \phi}{2}\right)$$

to directly get

$$\begin{aligned}
 &\frac{1}{2} \left( \cos\left(\frac{(2j-1)\pi}{n}\right) + \cos\left(\frac{(2j+1)\pi}{n}\right) \right) \\
 &= \cos\left(\frac{1}{2} \left[ \frac{(2j-1)\pi}{n} + \frac{(2j+1)\pi}{n} \right]\right) \cos\left(\frac{1}{2} \left[ \frac{(2j-1)\pi}{n} - \frac{(2j+1)\pi}{n} \right]\right) \\
 &= \cos\left(\frac{\pi}{n}\right) \cos\left(\frac{2j\pi}{n}\right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \frac{1}{n} \left[ \cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{2j\pi}{n}\right) \right] \\
 &= \frac{2}{n} \cos\left(\frac{1}{2} \left[ \frac{2j\pi}{n} + \frac{\pi}{n} \right]\right) \cos\left(\frac{1}{2} \left[ \frac{2j\pi}{n} - \frac{\pi}{n} \right]\right) \\
 &= \frac{2}{n} \cos\left(\frac{(2j-1)\pi}{2n}\right) \cos\left(\frac{(2j+1)\pi}{2n}\right).
 \end{aligned}$$

5: Directly computing, the characteristic polynomial is  $p(x) = \frac{1}{2}x(x-1)(2x^2 - 1)$ . The eigenvalues are  $1, \sqrt{2}/2, 0 - \sqrt{2}/2$  corresponding to  $\cos(0 \cdot \pi/4), \cos(1 \cdot \pi/4), \cos(2 \cdot \pi/4), \cos(3 \cdot \pi/4)$  respectively.

6: Consider the  $n \times n$  tridiagonal matrix

$$\begin{pmatrix} q & p & 0 & \cdots & 0 \\ q & 0 & p & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & q & 0 & p \\ 0 & \cdots & 0 & q & p \end{pmatrix}.$$

The equations connecting the eigenvalue  $\texttt{lambda}$  and the components  $u_i$  of the eigenvectors are

$$(21.1) \quad \texttt{lambda}u_1 = qu_1 + pu_2$$

$$(21.2) \quad \texttt{lambda}u_2 = qu_1 + pu_3$$

$$(21.3) \quad \vdots \quad \vdots$$

$$(21.4) \quad \texttt{lambda}u_{n-1} = qu_{n-2} + pu_n$$

$$(21.5) \quad \texttt{lambda}u_n = qu_{n-1} + pu_n.$$

Equations (.5) through (.7) are satisfied by  $u_j = s^j$  provided

$$\begin{aligned}
 \texttt{lambda}s^2 &= qs + ps^3 \\
 \vdots \quad \vdots \\
 \texttt{lambda}s^{n-1} &= qs^{n-2} + ps^n.
 \end{aligned}$$

These are all equivalent to  $\texttt{lambda}s = q + ps^2$ , or  $ps^2 - \texttt{lambda}s + q = 0$ , so the solutions are  $s_+ = \frac{\texttt{lambda} + \sqrt{\texttt{lambda}^2 - 4pq}}{2p}$  and  $s_- = \frac{\texttt{lambda} - \sqrt{\texttt{lambda}^2 - 4pq}}{2p}$ . Then

the solution is of the form

$$\begin{aligned} u_1 &= A(\text{lambda})s_+ + B(\text{lambda})s_- \\ u_2 &= A(\text{lambda})s_+^2 + B(\text{lambda})s_-^2 \\ &\vdots \\ u_{n-1} &= A(\text{lambda})s_+^{n-1} + B(\text{lambda})s_-^{n-1} \\ u_n &= A(\text{lambda})s_+^n + B(\text{lambda})s_-^n. \end{aligned}$$

Apply equation (.4) to get

$$\begin{aligned} \text{lambda}(As_+ + Bs_-) &= q(As_+ + Bs_-) + p(As_+^2 + Bs_-^2) \\ 0 &= A[(\text{lambda} - q)s_+ - ps_+^2] + B[(\text{lambda} - q)s_- - ps_-^2] \\ (21.6) \quad 0 &= A[q(s_+ - 1)] + B[q(s_- - 1)]. \end{aligned}$$

Applying the last equation (.8) to get

$$\begin{aligned} \text{lambda}(As_+^n + Bs_-^n) &= q(As_+^{n-1} + Bs_-^{n-1}) + p(As_+^n + Bs_-^n) \\ 0 &= As_+^{n-1}[(\text{lambda}s_+ - q) - ps_+] + Bs_-^{n-1}[(\text{lambda}s_- - q) - ps_-] \\ 0 &= As_+^{n-1}[ps_+^2 - ps_+] + Bs_-^{n-1}[ps_-^2 - ps_-] \\ (21.7) \quad 0 &= As_+^n p[s_+ - 1] + Bs_-^n p[s_- - 1] \\ (21.8) \quad -As_+^n p[s_+ - 1] &= Bs_-^n p[s_- - 1]. \end{aligned}$$

Substituting equation (.9) get

$$s_+^n = s_-^n.$$

Note that  $s_+s_- = q/p$  so  $s_+^{2n} = (q/p)^n$  and  $s_-^{2n} = (q/p)^n$ . That is, both  $s_+$  and  $s_-$  are  $(2n)$ th roots of  $(q/p)^n$ . Therefore,  $s_+$  and  $s_-$  can be written in the form

$$e^{i\pi j/n} = \sqrt{q/p} \left( \cos\left(\frac{\pi j}{n}\right) + i \sin\left(\frac{\pi j}{n}\right) \right)$$

for  $j = 0, 1, 2, \dots, 2n - 1$ .

Thus, the eigenvalues  $\text{lambda}$  are among the solutions of

$$s_+(\text{lambda}) = \sqrt{q/p} e^{i\pi j/n}$$



or

$$\begin{aligned}
\frac{\lambda + \sqrt{\lambda^2 - 4pq}}{2p} &= \sqrt{\frac{q}{p}} e^{i\pi j/n} \\
\lambda + \sqrt{\lambda^2 - 4pq} &= \sqrt{4pq} e^{i\pi j/n} \\
\sqrt{\lambda^2 - 4pq} &= -\lambda + e^{i\pi j/n} \\
\lambda^2 - 4pq &= \lambda^2 - 2\lambda \sqrt{4pq} e^{i\pi j/n} + 4pq e^{2i\pi j/n} \\
-4pq &= -2\lambda \sqrt{4pq} e^{i\pi j/n} + 4pq e^{2i\pi j/n} \\
\frac{4pq}{2\sqrt{4pq} e^{i\pi j/n}} + \frac{4pq e^{i\pi j/n}}{2\sqrt{4pq}} &= \lambda \\
\sqrt{4pq} \left( \frac{e^{-i\pi j/n}}{2} + \frac{e^{i\pi j/n}}{2} \right) &= \lambda \\
\sqrt{4pq} \cos \pi j/n &= \lambda.
\end{aligned}$$

So to each  $j$  there is a root  $\lambda_j$ , namely

$$\lambda_j = \sqrt{4pq} \cos(\pi j/n) \quad j = 0, 1, 2, \dots, 2n-1.$$

However, some of these roots are repeated, since

$$\cos(\pi j/n) = \cos(\pi(2n-j)/n)$$

for  $j = 1, \dots, n$ . So there are  $n$  eigenvalues  $\lambda_1 = 1$  and  $\lambda_j = \sqrt{4pq} \cos\left(\frac{(j-1)\pi}{n}\right)$  for  $j = 2, \dots, n$ . This is maximized for  $p = q = 1/2$ .

7: A simple R program using only base functions:

```

1 r <- 0
2 p <- 1/2
3 q <- 1 - p
4
5 for (n in 2:8) {
6
7   P <- diag(r, n, n)
8   P[ row(P) - col(P) == 1] <- p
9   P[ row(P) - col(P) == -1] <- q
10  P[1, 1] = q
11  P[n, n] = p
12
13  cat("Size of matrix: ", n, "Eigenvalues: ",
14      unlist(eigen(P, only.values=TRUE)), "\n")
15 }

```

1: Here the  $X$  process and the  $Y$  process definitely have different starting distributions. But the  $X$  process and the  $Y$  process both have the same (simple)

transition probabilities. To be explicit, suppose  $Y_0 = 0$ , and the first 5 transitions for  $Y$  are  $0 \rightarrow 1$ ,  $1 \rightarrow 1$ ,  $1 \rightarrow 1$ ,  $1 \rightarrow 0$ , and  $0 \rightarrow 1$ . Then the states are  $Y_0 = 0$ ,  $Y_1 = 1$ ,  $Y_2 = 1$ ,  $Y_3 = 1$ ,  $Y_4 = 0$ ,  $Y_5 = 1$ . By the definition of  $X_t$ ,  $X_0 = 0$ ,  $X_1 = Y_0 = 0$ ,  $X_2 = Y_1 = 1$ ,  $X_3 = Y_2 = 1$ ,  $X_4 = Y_3 = 1$ ,  $X_5 = Y_4 = 0$ . Then, for example

$$\mathbb{P}[X_{t+1} = 0 \mid X_t = 0] = \mathbb{P}[Y_t = 0 \mid Y_{t-1} = 0] = 1/2$$

and likewise for the other three transition probabilities. Thus,  $X_t$  also has transition probability matrix  $P$ . Furthermore, this same construction shows that  $(X_t, Y_t)$  is a Markov process on the 4-element state space. However

$$\mathbb{P}[X_1 = 0 \mid X_0 = 0, Y_0 = 0] = 1 \neq 1/2.$$

Essentially, the joint process is correct, but the marginals are not correct.

2:

## 21.12. Algorithms and Scripts

**Algorithm.**

**Scripts.**

## 21.13. Problems to Work for Understanding

1: Recall the magical land of Oz where the weather follows a pattern. If it is raining today, then tomorrow has a 50% chance of raining again, and a 25% chance of either having a nice day or a snowy day tomorrow. Similarly if it is snowing, the next day has a 50% chance of again having snow, and a 25% chance of either having a nice day, or a rainy day. Also the land of Oz never has two nice days in a row, and equally has rain or snow the day after a nice day. Recall that for  $P^n$ , for large values of  $n$ , the row vectors approach the stationary distribution  $\pi = (2/5, 1/5, 2/5)$ . Use the Theorem and Corollary to estimate the rate of convergence to the stationary of the Total Variation distance. Compare to the estimated rate of convergence using the Corollary and the eigenvalues of the transition probability matrix.



## Serial Chain Significance Testing

Following the work of Chikina, Frieze, Mattingly and Pegden [CFMP20, CFP17a, CFP19] this chapter derives statistical tests to detect that a given state from a stationary distribution of a reversible Markov chain is unusual. The *research hypothesis* is:

The given state is unusual with respect to a value measure.

Using a value function on the states of the Markov chain, this section rigorously bounds the probability that the given state is an outlier among the values. Doing so gives a  $p$  value for outliers, assuming the given state comes from the stationary distribution of the chain. The *null hypothesis* is:

The given state is not unusual with respect to a value measure.

In simplest form, the test is the following: Given a particular state in the Markov chain, take a random walk from the state for any number of steps. The simplest statistical test is finding the value of the presented state is an outlier on the walk with probability  $p \leq \sqrt{2\epsilon}$  assuming the state was from the stationary distribution. The test assumes nothing about the Markov chain beyond reversibility. With the simple serial test, probability at  $p \approx \sqrt{\epsilon}$  is the best possible in general. Compound tests in later sections using multiple random walks give improved probability of observing outlier values with  $p \approx \epsilon$ .

Mathematicians Only: prolonged scenes of intense rigor.

### 22.1. Chapter Starter Question

Given a statistical test for the null hypothesis that a state from a Markov chain is “not unusual” with respect to some function valuing the states, what would a *Type I error* for the statistical test mean?

Given a statistical test for the null hypothesis that a state from a Markov chain is “not unusual” with respect to some function valuing the states, what would a *Type II error* for the statistical test mean?

## 22.2. Background

An essential problem in statistics is to bound the probability of a surprising observation under the hypothesis that observations are drawn from some probability distribution. Often the bounding calculation is difficult. First, defining the way in which the outcome is surprising requires care. Second, the correct choice of the distribution for the hypothesis may not be immediately clear. Third, the  $p$  value calculations may be difficult even when the observation is surprising in a simple way and the hypothesis distribution is known but where there is no simple algorithm to draw samples from this distribution. In the third case, the best candidate method to sample under the hypothesis is often through a Markov chain, which essentially takes a long random walk among the possible values of the distribution. Under suitable conditions, theorems about Markov chains guarantee the chain converges to its stationary distribution, sometimes at a known rate, allowing a random sample to be drawn from a distribution quantifiably close to the target distribution. This principle is behind Markov chain Monte Carlo sampling and statistical physics models.

A problem in applications of Markov chains is the usually unknown rate at which the chain converges to the stationary distribution. It is rare to have rigorous results on the mixing time of a real-world Markov chain. In practice, sampling proceeds by running a Markov chain for a “long time” and hoping enough mixing has occurred.

In this section, the problem is assessing statistical significance in a Markov chain *without requiring information on the mixing time* of the chain or indeed, any special structure at all in the chain beyond reversibility. Consider a reversible Markov chain  $X$  on a state space  $\mathcal{X}$  with an associated value function  $v : \mathcal{X} \rightarrow \mathbb{R}$  (The notation here is  $v$  for the *value* function instead of  $\omega$  as in [CFP17a], to avoid overloading notation. Here  $\omega$  represents sample points in the sample space.) The values give auxiliary information without any relationship to the transition probabilities of  $X$ . The goal is to show a given state  $x_0$  is unusual for states drawn from the stationary distribution  $\pi$ . With good bounds on the mixing time of  $X$ , sampling  $v(x)$  from a distribution  $\pi$  gives a rigorous  $p$  value for the probability of the smallness of  $v(x_0)$ . However, such convergence bounds are rarely available.

Proposition 22.12 detects that  $X_0 = x_0$  is unusual relative to states chosen randomly according to  $\pi$ . The test does not need bounds on the mixing rate of  $X$ . First, a more precise definition of “unusual relative to states chosen randomly”.

**Definition 22.1.** A **value function**, also called a *label*, is a function  $v : \mathcal{X} \rightarrow \mathbb{R}$ . The value function has auxiliary information about the states of the chain and has no relationship to the transition probabilities of the Markov chain.  $\diamond$

**Remark 22.2.** For the statistical significance tests in this chapter the only relevant feature of the value function is the ranking it imposes on the elements of  $\mathcal{X}$ .

### 22.3. Outliers

**Definition 22.3.** A real number  $\alpha_0$  is an  $\epsilon$ -**outlier** among  $\alpha_0, \alpha_1, \dots, \alpha_n$  (not necessarily in increasing order and with repetitions possible) if there are, at most,  $\epsilon(n+1)$  indices  $i$  for which  $\alpha_i \leq \alpha_0$ , in other words  $\text{card}(\{\nu : \alpha_\nu \leq \alpha_0\}) \leq \epsilon(n+1)$ . Alternatively,  $\alpha_0$  is in the smallest  $\epsilon$ -fraction of the  $n+1$  ranked values of  $\alpha_0, \alpha_1, \dots, \alpha_n$ .  $\diamond$

**Remark 22.4.** For  $\alpha_0$  to be an  $\epsilon$ -outlier says  $\alpha_0$  is relatively more rare than the  $\epsilon$ -proportion that might be expected if the indices were uniformly distributed among the range of ranked values. For example, consider the set of 11 values

$$\alpha_0 = 3, \alpha_1 = 1, \alpha_2 = 4, \alpha_3 = 1, \alpha_4 = 5, \alpha_5 = 9, \\ \alpha_6 = 2, \alpha_7 = 6, \alpha_8 = 5, \alpha_9 = 3, \alpha_{10} = 5.$$

Then  $\alpha_0 = 3$  is *not* an 0.1-outlier since  $5 = \text{card}(\{\nu : \alpha_\nu \leq \alpha_0\}) \geq \epsilon(n+1) = 1.1$ . In fact,  $\alpha_0 = 3$  is *not* a 0.2-outlier (the cardinality is 5, greater than 2.2) or even a 0.3-outlier. This example says  $\alpha_0 = 3$  is not rare among small fractions of the values.

The following definition uses counting instead of proportions to express the smallness of a real number relative to a set. The proof of Proposition 22.12 uses this definition.

**Definition 22.5.** For  $1 \leq \ell \leq n+1$  say  $\alpha_j$  is **among- $\ell$ -smallest** in  $\alpha_0, \dots, \alpha_n$  if there are at most  $\ell$  indices from  $0, \dots, n$  such that  $\alpha_\nu$  is at most as large as  $\alpha_j$ . That is,  $\alpha_j$  is among- $\ell$ -smallest in  $\alpha_0, \dots, \alpha_n$  if

$$\text{card}(\{\nu : \alpha_\nu \leq \alpha_j\}) \leq \ell.$$

In particular,  $\alpha_j$  is among-1-smallest in  $\alpha_0, \dots, \alpha_n$  when its value is the unique minimum value.  $\diamond$

**Remark 22.6.** The definitions are connected:

- If  $\alpha_0$  is an  $\epsilon$ -outlier, then  $\alpha_0$  is among- $\lfloor \epsilon(n+1) \rfloor$ -smallest.
- If  $\alpha_0$  is among- $\ell$ -smallest, then  $\alpha_0$  is an  $\frac{\ell}{n+1}$ -outlier.

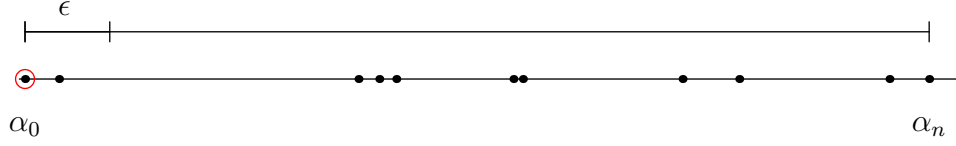
**Remark 22.7.** The definition of among- $\ell$ -smallest differs from the definition of  $\ell$ -small in [CFP17a]. Their definition excludes  $\alpha_j$  from the count, while the definition here includes  $\alpha_j$  in the count. The definition here corresponds with the definition of  $\epsilon$ -outlier which includes the value in question in the count.

**Example 22.8.** Consider the set of 11 real numbers drawn at random uniformly from  $[0, 1]$  and presented in sorted order:

$$0.006, 0.042, 0.359, 0.381, 0.399, 0.523, 0.533, 0.702, 0.762, 0.921, 0.963$$

so  $n = 10$  and let  $\epsilon = 0.1$ .

Then 0.006 is an 0.1-outlier since the number of indices for which  $\alpha_i \leq 0.006$ , specifically 1, is less than  $\epsilon(n+1) = 0.1 \cdot (10+1) = 1.1$ . See Figure 22.1 for an illustration of this example. However, 0.006 is not an 0.05-outlier since the number of indices for which  $\alpha_i \leq 0.006$ , specifically 1, is more than  $\epsilon(n+1) = 0.05 \cdot (10+1) = 0.55$ . As a further example, there are 2 indices for which  $\alpha_i \leq 0.042$  so 0.042 is not an 0.05, 0.1 or 0.15-outlier, but it is a 0.2-outlier



**Figure 22.1.** Example of  $\epsilon$ -outliers with 11 random values in  $[0, 1]$  and  $\epsilon = 0.1$ .

Also, 0.006 is among-1-smallest since there is 1 index from  $0, \dots, 10$  such that the value of  $\alpha_i$  is at most the value of 0.006. Additionally, 0.042 is among-2-smallest since there are 2 indices from  $0, \dots, 10$  such that the value of  $\alpha_i$  is at most the value of 0.042.

The notion of  $\epsilon$ -outlier is a generalization of median, quartile and percentile, see the exercises. The exercises also have a comparison of  $\epsilon$ -outlier and among- $\ell$ -smallest to the notions of the order of a list and the rank of elements of a list.  $\nabla$

## 22.4. Probability of Outliers

Proposition 22.12 gives an upper bound on the probability of a value of a Markov chain being among- $\ell$ -smallest using the following definition.

**Definition 22.9.** Let  $n$  be fixed. Let  $X_1, X_2, \dots, X_n$  be a sample of the Markov chain starting from  $X_0 = \sigma_0$ . Suppose the state space has a value function  $v : \mathcal{X} \rightarrow \mathbb{R}$ . For  $0 \leq j \leq n$  define

$$\rho(j; \ell, n) = \mathbb{P}[v(X_j) \text{ is among-}\ell\text{-smallest in } v(X_0), \dots, v(X_n)]$$

and

$$\rho(j; \ell, n \mid \sigma) = \mathbb{P}[v(X_j) \text{ is among-}\ell\text{-smallest in } v(X_0), \dots, v(X_n) \mid X_j = \sigma].$$

$\diamond$

When the value function  $v : \mathcal{X} \rightarrow \mathbb{R}$  is understood or not the focus of attention, for simplicity say  $X_j$  is among- $\ell$ -smallest among  $X_0, \dots, X_n$  instead of referring to the values of the states. Observe  $\rho(j; 1, n)$  is the probability  $X_j$  has the unique minimum value in the Markov chain of length  $n$ . Likewise,  $\rho(j; 1, n \mid \sigma)$  is the probability  $X_j = \sigma$  has the unique minimum value in the Markov chain of length  $n$  given that the Markov chain passes through  $\sigma$  at step  $j$ . Additionally,  $\rho(0; \ell, n \mid \sigma_0)$  is the probability that the starting value  $X_0 = \sigma_0$  is among- $\ell$ -smallest in  $v(X_0)$  through  $v(X_n)$ . Already these comments use the convention that the value function is omitted.

**Example 22.10.** The previous definitions have several levels:

- Markov chain sample paths of some length  $n$  with a value function,
- a upper bound  $\ell$ ,
- a specific step  $j$ ,
- the number of steps with value less than the given step, and
- the probability that number of steps is at most the upper bound.

step	0	1	2	3	4	5	6	7	8	9	10
1	5	4	4	3	3	4	4	4	4	3	3
2	2	2	3	4	4	3	4	3	2	3	4
3	3	3	3	2	3	2	2	3	3	4	4
4	3	3	3	2	3	2	3	4	4	3	4
5	5	5	6	5	5	4	4	4	3	3	4
6	4	4	4	4	4	3	4	5	4	4	5
7	3	3	3	4	5	6	5	4	3	3	4
8	4	4	4	4	4	5	4	4	4	4	4
9	4	5	5	5	4	4	4	4	4	5	4
10	4	5	5	4	5	4	4	5	5	4	5
11	4	4	3	3	2	3	3	4	3	2	2
12	3	3	3	3	2	3	3	3	2	2	3
13	2	3	2	2	1	0	1	2	2	3	2
14	1	2	3	4	5	6	6	6	5	4	5
15	5	6	7	6	5	4	4	5	6	6	5

**Table 22.1.** Record of 15 sample paths of the alternate Ehrenfest urn model.

This example illustrates those concepts of *among- $\ell$ -smallest* and  $\rho(j; 0, n)$  in the context of a specific Markov-chain.

Consider the alternative Ehrenfest urn model. Two urns, labeled  $A$  and  $B$ , contain a total of  $N = 7$  balls. At each step a ball is selected at random with all selections equally likely. Then an urn is selected, urn  $A$  with probability  $p = \frac{1}{2}$  and urn  $B$  with probability  $q = 1 - p = \frac{1}{2}$  and the ball is moved to that urn. The state at each step is the number of balls in the urn  $A$ , from 0 to  $N$ . Start from state  $\sigma$  selected at random from the stationary distribution. For this simple example, let the value function be the number of balls in urn  $A$ , so that the value function is identical with the state number. The simplicity of the alternative Ehrenfest urn model limits the possibilities for value functions.

This example uses the reproducible simulation of the alternate Ehrenfest urn model in `simRhoProb.R`. The path length, or number of steps, is 10, short enough to be comprehensible, long enough have some content. Including the start state, the Markov chain has 11 values. The number of trials is 15, enough to illustrate the variety of sample paths, but not too many to overwhelm. Thus the Markov chain is simulated 15 times starting from a state selected at random from the stable distribution. The values along the paths are recorded in the rows of an  $15 \times 11$  matrix. See Table 22.1. Then for each given step  $j$  along the path, the count of other step values along the path less than or equal to the given step value is compared to  $\ell$ . If the count is less than or equal to  $\ell$ , that makes the given step value at  $j$  among- $\ell$ -smallest and the count in a  $11 \times 11$  matrix is incremented. See Table 22.2. When done, divide the counting matrix entries by the number of trials, 15, to give an empirical estimate of  $\rho(j; \ell, n)$  with  $n = 11$ .

Next is a detailed analysis of Table 22.1 to illustrate the entries of the counting matrix in Table 22.2.



	1	2	3	4	5	6	7	8	9	10	11
0	1	1	2	2	4	5	6	7	10	12	15
1	0	1	2	2	3	3	3	4	6	10	15
2	0	0	1	1	2	2	3	5	8	10	15
3	0	1	2	3	5	5	5	7	9	12	15
4	0	0	3	4	4	5	6	8	10	13	15
5	2	4	5	5	6	7	9	10	10	11	15
6	0	1	3	3	4	5	6	8	9	12	15
7	0	0	0	0	0	2	4	5	7	9	15
8	0	1	3	3	4	4	5	7	10	13	15
9	0	1	3	4	7	7	8	9	10	12	15
10	0	0	1	2	2	4	5	7	8	9	15

Table 22.2. The count of step values

- The entry at  $[0, 1]$  records the number of trials where the starting value  $j = 0$  is the unique minimum. In trials 2, 7, 8, 9, 10 the start value is the minimum of the path, but not the unique minimum. In trial 14, the start value 1 is the unique minimum, which gives the entry value 1.
- Entries at  $[j, 1]$ , with  $j \geq 1$ , record the number of trials where the value of step  $X_j$  is the unique minimum. In trial 6, at step  $j = 5$  and in trial 13, at step  $j = 5$  the unique minimum occurs. Thus the  $[5, 1]$  entry is 2.
- The entry at  $[0, 1]$  records the number of trials where the start value, namely  $X_0$ , is among-1-smallest. That is, the number of trials where the number of values less than or equal to the start value is less than or equal to 1. This is just trial 14 again.
- The entry at  $[0, 2]$  records the number of trials where the start value  $X_0$  is among-2-smallest. That is, the number of trials where the number of values less than or equal to the start value is less than or equal to 2. This is just trial 14 again, with no other values less than  $X_0 = 1$ .

See the exercises for more explanation of entries in Table 22.2.

This example is deliberately small in scope to illustrate the definition of  $\rho(j; \ell, n)$ . Increasing the path length and the number of trials gives better empirical estimates for  $\rho(j; \ell, n)$ .  $\nabla$

**Remark 22.11.** For a given value of  $n$ ,  $\rho(j; \ell, n)$  is increasing in  $\ell$  like a c.d.f. This is an obvious conclusion, since the definition is in terms of an inequality and gets more permissive in terms of the number of allowed values in the among- $\ell$ -smallest.

**Proposition 22.12.** (1) Fix  $n$ .

- (2) Suppose  $X_0$  is chosen from the stationary distribution  $\pi$  of the reversible Markov chain  $X$ .
- (3) Suppose  $X_1, X_2, \dots, X_n$  is a sample of the Markov chain starting from  $X_0$ .
- (4) Suppose the state space has a value function  $v : \mathcal{X} \rightarrow \mathbb{R}$ .
- (5) Let

$$\rho(j; \ell, n) = \mathbb{P}[v(X_j) \text{ is among-}\ell\text{-smallest in } v(X_0), \dots, v(X_n)].$$

Then

$$\rho(0; \ell, n) \leq \sqrt{\frac{2\ell - 1}{n + 1}}.$$

**Proof.** (1) For simplicity, omit the value function in the proof and just say  $\rho(j; \ell, n) = \mathbb{P}[X_j \text{ is among-}\ell\text{-smallest in } X_0, \dots, X_n]$ . For a first understanding of the proof, use the  $\ell = 1$  case, so the minimum value is the focus.

(2) Let  $\pi$  denote the stationary distribution for  $X$  and suppose the initial state  $X_0$  is distributed as  $X_0 \sim \pi$ , so that in fact,  $X_\nu \sim \pi$  for all  $\nu$ .

(3) Observe that because  $X_s \sim \pi$  for all  $s$ , additionally

$$\begin{aligned} \rho(j; \ell, n \mid \sigma) &= \\ &\mathbb{P}[X_{s+j} \text{ is among-}\ell\text{-smallest in } X_s, \dots, X_{s+n} \mid X_j = \sigma]. \end{aligned}$$

(4) Because  $X = X_0, X_1, \dots$  is stationary and reversible, the probability of  $(X_0, \dots, X_n) = (\sigma_0, \dots, \sigma_n)$  equals the probability  $(X_0, \dots, X_n) = (\sigma_n, \dots, \sigma_0)$  for any fixed sequence  $(\sigma_0, \dots, \sigma_n)$ . Thus, any sequence  $(\sigma_0, \dots, \sigma_n)$  for which  $\sigma_j = \sigma$  and  $\sigma_j$  is a among- $\ell$ -smallest corresponds to an equiprobable sequence  $(\sigma_n, \dots, \sigma_0)$ , for which  $\sigma_{n-j} = \sigma$  and  $\sigma_{n-j}$  is among- $\ell$ -smallest. Thus a first fact about  $\rho(j; \ell, n \mid \sigma)$  for reversible Markov chains is:

$$\rho(j; \ell, n \mid \sigma) = \rho(n - j; \ell, n \mid \sigma).$$

(5) The next claim is:

$$\rho(j; 2\ell - 1, n \mid \sigma) \geq \rho(j; \ell, j \mid \sigma) \cdot \rho(0; \ell, n - j \mid \sigma).$$

The proof of the claim is to consider a first event that  $X_j$  is among- $\ell$ -smallest in  $X_0, \dots, X_j$  and a second event that  $X_j$  is among- $\ell$ -smallest in  $X_j, \dots, X_n$ . The first term  $\rho(j; \ell, j \mid \sigma)$  is the probability that  $X_j$  is among- $\ell$ -smallest of the  $j + 1$  values from  $X_0$  to  $X_j$ . The second term  $\rho(0; \ell, n - j \mid \sigma)$  is the probability that  $X_j$  is among- $\ell$ -smallest of the  $n - j$  values from  $X_j$  to  $X_n$ . These events are conditionally independent when conditioning on the value of  $X_j = \sigma$ , which allows taking the product. When both of these events happen, then  $X_j$  is among- $2\ell - 1$ -smallest in  $X_0, \dots, X_n$ , with  $2\ell - 1$  because  $X_j$  was counted in each event. Both events happening is a subevent of the desired event of  $X_j$  being among- $2\ell - 1$ -smallest from  $X_0$  to  $X_n$ . This establishes the inequality in the claim.

(6) Using the previous steps

$$\begin{aligned} \rho(j; 2\ell - 1, n \mid \sigma) &\geq \rho(j; \ell, j \mid \sigma) \cdot \rho(0; \ell, n - j \mid \sigma) \\ &= \rho(0; \ell, j \mid \sigma) \cdot \rho(0; \ell, n - j \mid \sigma) \\ &\geq (\rho(0; \ell, n \mid \sigma))^2. \end{aligned}$$

where the first inequality comes from step 5. The middle equality comes from step 4. The last inequality comes from the simple observation that  $\rho(j; \ell, n \mid \sigma)$  is nonincreasing in  $n$  for fixed  $j, \ell$  and  $\sigma$ , in particular for  $j$  fixed to be 0.

- (7) Now  $\rho(j; \ell, n) = \mathbb{E}[\rho(j; \ell, n \mid \sigma)]$ , where the expectation is taken over the random choice of  $\sigma \sim \pi$ . Thus, taking expectations over the inequality in step 6,

$$(22.1) \quad \begin{aligned} \rho(j; 2\ell - 1, n) &= \mathbb{E}[\rho(j; 2\ell - 1, n \mid \sigma)] \geq \mathbb{E}[\rho(j; \ell, n \mid \sigma)^2] \\ &\geq (\mathbb{E}[\rho(0; \ell, n \mid \sigma)])^2 = (\rho(0; \ell, n))^2 \end{aligned}$$

where the second of the two inequalities is the Cauchy-Schwartz inequality.

- (8) To complete the proof, sum the left- and right-hand sides of the inequality in step 7

$$\sum_{j=0}^n \rho(j; 2\ell - 1, n) \geq (n+1)(\rho(0; \ell, n))^2.$$

- (9) Letting  $\mathbf{1}_j$ ,  $0 \leq i \leq n$  be the indicator variable that is 1 whenever  $X_j$  is among- $2\ell - 1$ -smallest in  $X_0, \dots, X_n$ , then  $\sum_{\nu=0}^n \mathbf{1}_\nu$  is the number of among- $2\ell - 1$ -smallest terms, which is at most  $2\ell$ . Therefore, linearity of expectation gives

$$2\ell - 1 \geq (n+1)(\rho(0; \ell, n))^2$$

so

$$\rho(0; \ell, n) \leq \sqrt{\frac{2\ell - 1}{n+1}}.$$

□

**Remark 22.13.** Proposition 22.12 only gives a theoretical upper bound for  $\rho(0; \ell, n)$  although the alternate Ehrenfest urn model simulation gives empirical estimates for all  $\rho(j; \ell, n)$ . The theoretical upper bound is not very sharp either, for instance  $\rho(0; n, n) = 1$ , but the theoretical upper bound is approximately  $\sqrt{2}$ .

**Remark 22.14.** Proposition 22.12 can only show a given sample is unusual with respect to  $\pi$ . The Proposition does not give a way to generate samples from  $\pi$ .

**Remark 22.15.** The Proposition makes no assumptions on the structure of the Markov chain beyond reversibility. If a Markov chain can be broken down into two disjoint communicating classes, i.e. two disconnected Markov chains and if the individual Markov chains are reversible, then so is the full chain. This is a worthwhile observation, since all examples of reversible Markov chains so far are irreducible, giving the wrong impression that all reversible Markov chains are irreducible.

In particular, the Proposition applies even if the chain is not irreducible, i.e. even if the state space is not connected under the Markov chain. In this disconnected case the chain will never completely mix since it remains in one component. This remark is important for the example application below of Markov chains sampling valid political districting, where it is not known that the Markov chains are irreducible. Even if valid districting only requires contiguous districts of roughly equal populations, it is unknown if any valid districting is reachable from any other by a legal sequence of steps.

This suggests a careful choice of value function can help to distinguish irreducible components, especially in political districting. Suppose one component is

relatively small and unusual compared to more typical states from a larger component. A value function measuring this difference would be a candidate for the Proposition.

**Corollary 22.16** (The  $\sqrt{2\epsilon}$  Test). (1) Fix  $n$ .

(2) Suppose  $X_0$  is chosen from the stationary distribution  $\pi$  of the reversible Markov chain  $X$ .

(3) Suppose  $X_1, X_2, \dots, X_n$  is a sample of the Markov chain starting from  $X_0$ .

(4) Suppose the state space has a value function  $v : \mathcal{X} \rightarrow \mathbb{R}$ .

Then the event  $v(X_0)$  is an  $\epsilon$ -outlier among  $v(x_0), \dots, v(x_n)$  with probability  $p = \sqrt{2\epsilon}$ .

**Proof.** (1) The reversible Markov chain  $X$ , the stationary distribution  $\pi$ , the value function  $v$ , fixed integer  $n$ , and fixed small proportion  $\epsilon$  determine a  $n$ -vector  $(\rho(0; \epsilon, n), \rho(1; \epsilon, n), \dots, \rho(n; \epsilon, n))$  where, with a slight abuse of notation, for each  $i$ ,  $\rho(i; \epsilon, n)$  is the probability that in a  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_n$ ,  $v(X_i)$  is among  $\lfloor \epsilon(n+1) \rfloor$ -smallest in the list  $v(X_0), v(X_1), \dots, v(X_n)$ .

(2) Proposition 22.12 proves

$$\rho(0; \epsilon, n) \leq \sqrt{\frac{2\lfloor \epsilon(n+1) \rfloor - 1}{n+1}} \leq \sqrt{\frac{2\epsilon(n+1) - 1}{n+1}} \leq \sqrt{2\epsilon}.$$

□

**Remark 22.17.** This is a restatement of Proposition 22.12 as a statistical test in terms of the proportion  $\epsilon$ .

**Remark 22.18.** Chikina, et al. [CFP17a] call Corollary 22.16 the  $\sqrt{\epsilon}$  test, but this section slightly revises their terminology. Corollary 22.16 could be called either the  $\epsilon$  test, referring to the outlier fraction, or the  $\sqrt{2\epsilon}$  Test referring to the significance level. Looking ahead to more refined tests, call Corollary 22.16 the  $\sqrt{2\epsilon}$  test for serial or sequential Markov chain samples.

**Remark 22.19.** The Type I error rate is the probability of rejecting the null hypothesis, given the null hypothesis is true. See Figure 22.2 for a diagram of possible decisions about the null hypothesis and possible errors in the decision. Corollary 22.16 says if the value is an  $\epsilon$ -outlier, then the probability of *erroneously* concluding  $X_0$  is *not unusual*, when in fact  $X_0$  is unusual, is less than  $\sqrt{2\epsilon}$ .

An example later shows the relationship  $p \approx \sqrt{\epsilon}$  is best possible. It is currently an open question whether the constant 2 can be improved.

**Remark 22.20.** The power of a binary null hypothesis test is the probability the test correctly rejects the null hypothesis when the alternative hypothesis is true. The power is the complementary probability of a Type II error. Here the power is the probability the  $\sqrt{2\epsilon}$  Test correctly says  $X_0$  as an  $\epsilon$ -outlier is unusual. Later sections consider the statistical power of the  $\sqrt{2\epsilon}$  Test.

Error Types		Null hypothesis is	
		True	False
Decision	Don't reject	Correct Inference	Type II error
	Reject	Type I error	Correct Inference

**Figure 22.2.** Tabular presentation of hypothesis testing, decisions and error types.

Another way to look at the  $\sqrt{2\epsilon}$  Test is the following. The Markov chain  $X$ , the stationary distribution  $\pi$ , the valuing  $v$ , and a fixed integer  $n$  determine a  $n$ -vector  $(p_0^n, p_1^n, \dots, p_n^n)$  where for each  $\nu$ ,  $p_\nu^n$  is the probability that in a  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_n$ , the minimum  $v$  value occurs at  $X_i$ . In other words, choosing  $X_0$  randomly from the stationary distribution  $\pi$  and taking  $n$  steps in  $\mathcal{X}$  to obtain the trajectory  $X_0, X_1, \dots, X_n$ , the probability that observing  $v(X_i)$  is the minimum among  $v(X_0), v(X_1), \dots, v(X_n)$  is  $p_i^n$ . Adopt the convention that ties for minimum among the values  $v(X_0), v(X_1), \dots, v(X_n)$  picks  $i$  randomly (uniformly among the steps achieving the minimum) so  $p_0^n + p_1^n + \dots + p_n^n = 1$  for  $X, \pi, n$ .

Thinking the minimum value is roughly equally likely to occur anywhere in the chain, it might be natural to guess  $p_i^n \approx \frac{1}{n+1}$ . To be the minimum value means the value occurs in the least  $\frac{1}{n+1}$  fraction, so  $\epsilon = \frac{1}{n+1}$ . Corollary 22.12 shows  $p_0^n \leq \frac{1}{\sqrt{n+1}}$ . The next section has an example that  $p_0^n$  can be as large as  $\frac{1}{\sqrt{2\pi n}}$ . The

example means the  $O(\sqrt{\epsilon})$  probability from Corollary 22.16, as the worst possible behavior for  $p_0^n$ , can actually be achieved.

In the general setting of a reversible Markov chain, the Corollary leads to a simple quantitative procedure for asserting rigorously  $\sigma_0$  is atypical with respect to  $\pi$  without knowing the mixing time of  $X$ : simply observe a random trajectory  $\sigma_0 = X_0, X_1, X_2, \dots, X_n$  from  $\sigma_0$  for any fixed  $n$ . If  $v(\sigma_0)$  is an  $\epsilon$ -outlier among  $v(X_0), v(X_1), \dots, v(X_n)$ , then the probability of *erroneously* concluding  $X_0$  is *not unusual*, when in fact the null hypothesis that  $X_0$  is not unusual is true, is less than  $\sqrt{2\epsilon}$ .

Corollary 22.16 leads to the *Outlier Test Algorithm*:

**Data:** Markov chain  $X$ , starting state  $X_0$ , value function  $v(\cdot)$

**Result:** probability  $\sqrt{2\epsilon}$  of *erroneously* concluding  $X_0$  is *not unusual* with respect to the value function.

- 1 Begin from the state being evaluated for “outlier” status.
- 2 Make a sequence of  $n$  random changes to the states according to the Markov chain transition probabilities.
- 3 Evaluate the labeling of the chain.
- 4 Call the original state an “outlier” if the overwhelming majority of values (more than  $1 - \epsilon$  of the values) are greater in value than the starting state.

**Algorithm 20:** Outlier Test Algorithm.

**Remark 22.21.** The Outlier Test Algorithm is useful because  $\sqrt{2\epsilon}$  is reasonably close to 0 for  $\epsilon$  small; in particular, it is possible to obtain “good enough” statistical significance from observations which can be made with reasonable computational resources. Of course, smaller probability compared to  $\epsilon$  would be even better, but, as already noted,  $p = O(\sqrt{\epsilon})$  is the best possible with a single serial Markov chain.

**Remark 22.22.** The  $\sqrt{2\epsilon}$ -Test is a simple informal interpretation for the general behavior of reversible Markov chains. Specifically, the long-term typical states are unlikely (with  $p = O(\sqrt{\epsilon})$ ) to differ in a measurable way (be in the smallest  $\epsilon$  fraction measured by the value) under a sequence of chain transitions, with a best-possible quantification up to constant factors.

Next is a corollary of Proposition 22.12 that applies to the setting where  $X_0$  is not distributed as the stationary distribution  $\pi$  but instead is distributed with small total variation distance to  $\pi$ .

**Corollary 22.23.** (1) Let  $X$  be a reversible Markov chain on  $\mathcal{X}$ .

(2) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(3) Let  $X_0$  be a state chosen from  $\text{dist}(\mathcal{X})$  with distribution such that

$$\|\text{dist}(\mathcal{X}) - \pi\|_{TV} \leq \epsilon_1.$$

Then for any fixed  $n$ , the probability the value of  $X_0$  is an  $\epsilon$ -outlier from among the list of values observed in the trajectory  $X_0, X_1, \dots, X_n$  is at most  $\sqrt{2\epsilon} + \epsilon_1$

- Proof.** (1) If  $\rho_1$ ,  $\rho_2$ , and  $\rho_3$  are probability distributions, then the product distributions  $(\rho_1, \rho_3)$  and  $(\rho_2, \rho_3)$  satisfy  $\|(\rho_1, \rho_3) - (\rho_2, \rho_3)\|_{TV} = \|\rho_1 - \rho_2\|_{TV}$ . See the exercises.
- (2) Split the randomness in the trajectory  $X_0, \dots, X_n$  of the Markov chain into two independent sources: the initial distribution is  $X_0 \sim \text{dist}(\mathcal{X})$ , and  $U$  is the uniform distribution on sequences of length  $n$  of real numbers  $r_1, r_2, \dots, r_n$  in  $[0, 1]$ .
- (3) The distribution of the trajectory  $X_0, X_1, \dots, X_n$  is the product  $(\rho, U)$  by using sequences of reals  $r_1, \dots, r_n$  to choose transitions in the chain; from  $X_i = \sigma_i$ , if there are  $L$  transitions possible, with probabilities  $p_1, \dots, p_L$ .
- (4) Then, make the  $t$ th possible transition if  $r_i \in [p_1 + \dots + p_{t-1}, p_1 + \dots + p_{t-1} + p_t]$ . If  $\|\text{dist}(\mathcal{X}) - \pi\|_{TV} \leq \epsilon_1$ , then  $\|(\text{dist}(\mathcal{X}), U) - (\pi, U)\|_{TV} \leq \epsilon_1$ .
- (5) Therefore, any event that would happen with probability at most  $p$  for the sequence  $X_0, \dots, X_n$  when  $X_0 \sim \pi$  must happen with probability at most  $p + \epsilon_1$  when  $X_0 \sim \rho$ , where  $\|\rho - \pi\|_{TV} \leq \epsilon_1$ . The corollary follows.  $\square$

## 22.5. Simple Example of Unusual States

**Example 22.24.** Consider a specific simple case of the alternative Ehrenfest urn model. The setup of the urn model is repeated here for convenient reference. Two urns, labeled  $A$  and  $B$ , contain a total of  $N = 7$  balls. At each step a ball is selected at random with all selections equally likely. Then an urn is selected, urn  $A$  with probability  $p = \frac{1}{2}$  and urn  $B$  with probability  $q = 1 - p = \frac{1}{2}$  and the ball is moved to that urn. The state at each step is the number of balls in the urn  $A$ , from 0 to  $N$ . Start from state 0, with no balls in urn  $A$ . All states are accessible and all states communicate, so the chain is irreducible. All states are recurrent and there are no transient states. The chain is periodic with period 1 so it is regular. The standard Ehrenfest urn model, without the random choice of urns at each step, is periodic with period 2. Having period 1 makes interpretation of the results simpler.

For this simple example, let the value function be the number of balls in urn  $A$ , so that the value function is identical with the state number. The simplicity of the alternative Ehrenfest urn model limits the possibilities for value functions. More interesting value functions appear in the gerrymandering example later, where the states have considerably more structure and information associated with them.

The second largest (in absolute magnitude) eigenvalue of the transition probability matrix is approximately 0.857. The total variation distance of the probability distribution of the states at step  $n$  should differ from the stationary distribution by a multiple of  $(0.857)^n$ . Therefore, it takes about 30 steps for the total variation distance of the probability distribution of the states to differ from the stationary distribution by less than 0.01. For the alternative Ehrenfest urn model with 7 balls, the stationary distribution of the Markov chain started from state 0 will be in state 0 about 0.78125% of the steps. In 199 steps, together with the starting state 0, it would be typical to see the state 0 just once or twice. Equivalently, the mean recurrence time to state 0 is 128 steps, so again in 199 steps it would be typical to see the state 0 just once or twice. This shows the state 0 is an unusual state with

respect to the stationary distribution, which also should be expected from the statistical mechanical interpretation of the alternative Ehrenfest urn model. The state 0 is a state of high statistical-mechanical order, with all the balls in urn  $B$ , none in urn  $A$ . Such highly ordered states should be unlikely. In summary, the value 0 should be fairly unusual, in spite of 0 being a state in the stationary distribution.

If  $\epsilon = 0.01$ , then this analysis predicts that value 0 would usually be an  $\epsilon$ -outlier for the set of values generated by the chain, since it would usually appear in the smallest  $\epsilon$ -fraction of the 200 ranked values, that is, the least two values. Equivalently 198 of the 200 values from the path would be greater than 0. Actually running simulations of the alternative Ehrenfest Markov chain shows state 0 is an 0.01-outlier according to this test about half of the time, see the exercises. The simulations show that rejecting the null hypothesis, that is, concluding in error that 0 is *not unusual* with respect to the stationary distribution, occurs about half the time.

However, with just 8 values, there is not much to distinguish being an  $\epsilon$ -outlier, and sampling variation among Markov chain runs could account for false negatives, that is, finding the truly unusual state 0 (unusual in the sense of high statistical-mechanical order and unusual in the sense of infrequent visitation) occurs in the larger  $1 - \epsilon$  fraction of the values, asserting that value 0 is not unusual. Experiments with more trials with longer path lengths for the Markov chain shows the proportion of trials showing 0 is an  $\epsilon$ -outlier, that is, the empirical probability, slowly increases. Rejecting the null hypothesis increases with increasing the length of the chain, as expected. This is an illustration of the problem of determining the statistical power of the test discussed later.

Considering larger specific cases of the alternative Ehrenfest urn model with  $N = 21$  and  $N = 51$  balls illustrates the utility of a more discriminating value function. With  $N = 21$  balls, Markov chain runs of 399 steps in 400 trials the proportion showing 0 is an  $\epsilon$ -outlier is about 0.92. With longer Markov chain runs of 800 or 1600 steps in 1000 trials, the proportion showing 0 is an  $\epsilon$ -outlier is better than 0.97. With  $N = 51$  balls, the probability of showing state 0 is unusual in long runs is virtually certain.

The important observation is that with a sufficiently long run, and a sufficiently discriminating value function, the  $\epsilon$ -outlier test can show state 0 is unusual with high confidence without knowing the mixing time, or that the Markov chain is in the steady state, or even the steady state distribution.

▽

## 22.6. Example Where $p = O(\sqrt{\epsilon})$ Is the Best Possible

It might be natural to suspect that observing  $\epsilon$ -outlier status for  $\sigma$  on a random trajectory from  $\sigma$  is significant at  $p = O(\epsilon)$  instead of the probability  $p = O(\sqrt{\epsilon})$  established by Corollary 22.16. However, because Corollary 22.16 uses no information about the mixing rate of  $X$  or the stationary distribution, it seems remarkable any significance can be shown in general. An example in this section shows probability at  $p = O(\sqrt{\epsilon})$  is the best possible.



Given  $n$  and  $\epsilon$ , choose  $N > \frac{2n+1}{\epsilon}$ . Let  $X$  be the Markov chain where  $X_0$  is chosen at random uniformly in  $\mathcal{X} = \{0, 1, 2, \dots, N-1\}$ , and for any  $\nu \geq 1$ ,  $X_\nu$  is equal to  $X_{\nu-1} + \zeta_\nu$  modulo  $N$ , where  $\zeta_\nu = \pm 1$  with equal probability  $\frac{1}{2}$ . That is,  $X$  is random walk on the circle. Note the chain is reversible and has stationary distribution  $\pi_\nu = \frac{1}{N}$ . The value function is the position around the circle, that is,  $v(X_\nu) = X_\nu$ .

Then  $N$  is large enough that the distance of  $X_0$  from 0 in both directions is greater than  $n$  with probability greater than  $1 - \epsilon$ . Conditioning on this event,  $X_0$  is minimum, i.e. among-1-smallest in  $X_0, \dots, X_n$  if and only if all of the partial sums  $\sum_{\nu=1}^j \zeta_\nu$  are positive for  $j \leq n$ . The probability of this event is just the probability an  $n$ -step 1-dimensional random walk from  $X_0$  takes a first step to the right and does not return to the origin. The calculation of this probability is a classical problem in random walks, solved using the reflection principle. In particular, for  $n$  even, the probability is given exactly by (see the exercises)

$$\frac{1}{2^{n+1}} \binom{n}{n/2} \sim \frac{1}{\sqrt{2\pi n}}.$$

Because being the minimum or among-1-smallest of  $X_0, \dots, X_n$  corresponds to being an  $\epsilon$ -outlier for  $\epsilon = \frac{1}{n+1}$  this example shows the probability of being an  $\epsilon$ -outlier can be as high as (a nearly unit multiple of)  $\sqrt{\epsilon/(2\pi)}$ . Of course,  $\sqrt{\epsilon/(2\pi)} < \sqrt{2\epsilon}$  so the best possible value of the constant in the  $\sqrt{2\epsilon}$  test is an interesting question.

Figure 22.3 schematically illustrates a specific example. Let  $n = 198$ ,  $\epsilon = 0.01$ , so  $N > \frac{2n+1}{\epsilon} = 39,700$ . Take  $N = 40,000$  for simplicity. States, such as 20,000, chosen outside the region marked with bars have the distance of  $X_0$  from 0 in both directions is greater than  $n = 198$  with probability greater than  $1 - \epsilon = 0.99$ . An  $n$ -step random walk from  $X_0$  satisfying the condition is drawn schematically.

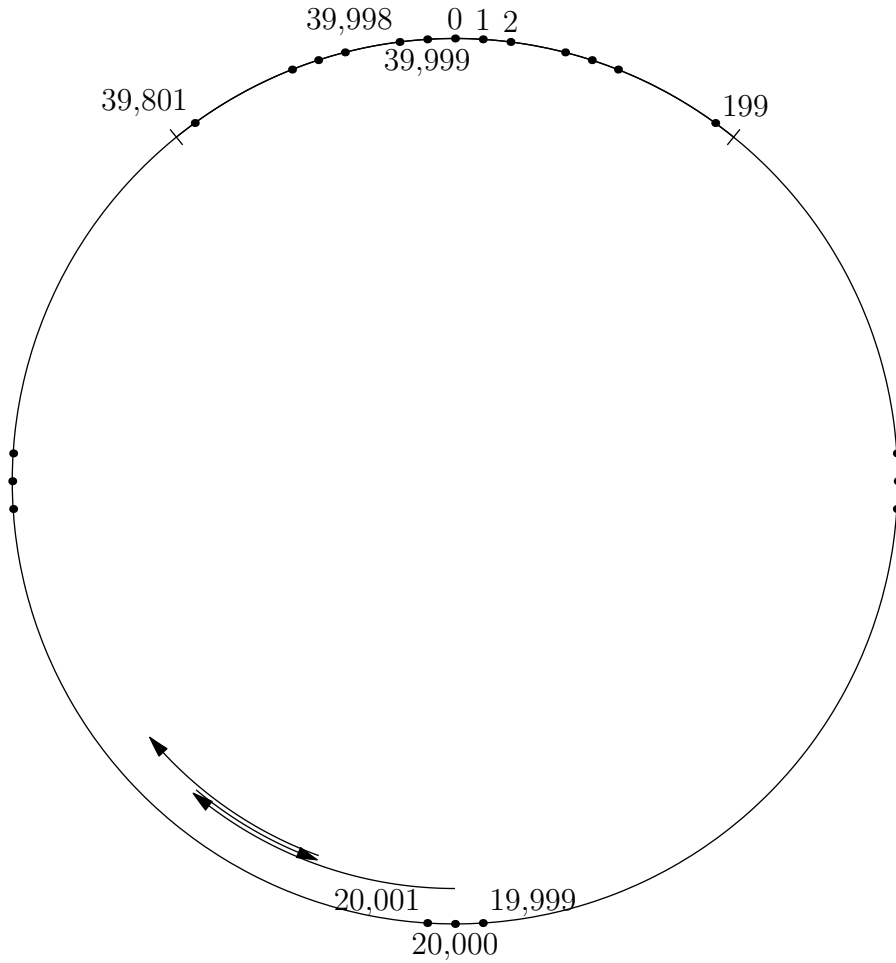
## 22.7. Notes on Statistical Power

The effectiveness of the  $\sqrt{2\epsilon}$  test depends on the availability of a sufficiently discriminating choice for the value function  $v$  and the ability to run the test for long enough (in other words, choose  $n$  large enough) to detect the presented state is an  $\epsilon$ -outlier. It is possible, however, to make a general statement about the power of the test when  $n$  is chosen large relative to the actual mixing time of the chain. Recall one potential application of the test is in situations where the mixing time of the chain is actually accessible through reasonable computational resources, although this fact cannot be proved rigorously, because theoretical bounds on the mixing time are often not available. In particular, the test is very likely to succeed when  $n$  is sufficiently large and  $v(\sigma_0)$  is unusual as already shown by the alternative Ehrenfest urn model.

**Remark 22.25.** Let  $\tau_{\text{rel}}$  be the *relaxation time* for  $X$  defined as  $1/(1 - \beta_*)$  where

$$\beta_* = \max \{|\beta| : \beta \text{ is an eigenvalue of } P, \beta \neq 1\}$$

is the *absolute spectral gap* for  $X$ . The relaxation time is related to the mixing time of  $X$ . Let  $d(t) = \sup_\sigma \|P^t - \pi\|_{TV}$ . The *mixing time* is  $\tau_{\text{mix}}(\epsilon) = \min \{t : d(t) \leq \epsilon\}$ .



**Figure 22.3.** A schematic diagram of the random walk on a circle illustrating the example of the best possible bound.

For reversible chains [LPW09, Theorems 12.3, 12.4],

$$(\tau_{\text{rel}} - 1) \log \left( \frac{1}{2\epsilon} \right) \leq \tau_{\text{mix}}(\epsilon) \leq \tau_{\text{rel}} \log \left( \frac{1}{\epsilon \min_x \pi(x)} \right).$$

In some cases the relaxation time can be calculated from the eigenvalues of the transition probability matrix to give bounds on the mixing time. Typically, the mixing time is difficult to find directly.

Theorem 22.27 below is a simple application of the following theorem of Gillman [Gil98, Theorem 2.1] translated into the current notation and assumptions.

**Theorem 22.26** (Gillman’s Chernoff-Type Bound). (1) Let  $X$  be a reversible Markov chain on  $\mathcal{X}$ .

(2) Let  $A \subset \mathcal{X}$ .

(3) Let  $N_n(A)$  denote the number of visits to  $A$  among  $X_0, X_1, \dots, X_n$ .

Then for any  $\gamma > 0$ ,

$$\mathbb{P}[N_n(A)/n - \pi(A) \geq \gamma] \leq \left(1 + \frac{\gamma}{10\tau_{\text{rel}}}\right) \sqrt{\sum_{\sigma} \frac{(\mathbb{P}[X_0 = \sigma])^2}{\pi(\sigma)}} \exp\left(\frac{-\gamma^2 \cdot n}{20\tau_{\text{rel}}}\right).$$

**Proof.** To be added. See [Gil98]. □

**Theorem 22.27.** (1) Let  $X$  be a reversible Markov chain on  $\mathcal{X}$ .

(2) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(3) Given  $X_0$ , suppose for a random state  $X \sim \pi$ ,

$$\mathbb{P}[v(X) \leq v(X_0)] \leq \epsilon.$$

Then with probability  $p$ , where

$$p \geq 1 - \left(1 + \frac{\epsilon}{10\tau_{\text{rel}}}\right) \cdot \frac{1}{\sqrt{\pi_{\min}}} \cdot \exp\left(\frac{-\epsilon^2 \cdot n}{20\tau_{\text{rel}}}\right),$$

$v(X)$  is a  $2\epsilon$ -outlier among  $v(X_0), v(X_1), \dots, v(X_n)$  where  $X_0, X_1, \dots, X_n$  is a random trajectory starting from  $X_0$ .

**Proof.** (1) Apply Theorem 22.26 with  $A$  as the set of states  $\sigma \in \mathcal{X}$  such that  $v(\sigma) \leq v(X_0)$ ,  $X_0 = \sigma_0$  and  $\gamma = \epsilon$ . By Hypothesis 3  $\pi(A) \leq \epsilon$ .

(2) Theorem 22.26 gives

$$\mathbb{P}[N_n(A)/n > 2\epsilon] \leq \left(1 + \frac{\epsilon}{10\tau_{\text{rel}}}\right) \cdot \frac{1}{\sqrt{\pi_{\min}}} \cdot \exp\left(\frac{-\epsilon^2 \cdot n}{20\tau_{\text{rel}}}\right).$$

(3) The proof uses the additional simplification:

$$\frac{(\mathbb{P}[X_0 = \sigma])^2}{\pi(\sigma)} \leq \frac{(\mathbb{P}[X_0 = \sigma])^2}{\pi_{\min}}$$

so

$$\sum_{\sigma} \frac{(\mathbb{P}[X_0 = \sigma])^2}{\pi(\sigma)} \leq \sum_{\sigma} \frac{(\mathbb{P}[X_0 = \sigma])^2}{\pi_{\min}} \leq \frac{(\sum_{\sigma} \mathbb{P}[X_0 = \sigma])^2}{\pi_{\min}} = \frac{1}{\pi_{\min}}$$

using standard inequalities. □

**Remark 22.28.** The probability  $p$  in Theorem 22.27 converges in  $n$  exponentially quickly to 1. The probability  $p$  is very close to 1 if  $n$  is large relative to  $\tau_{\text{rel}}$ . In particular, Theorem 22.27 shows the  $\sqrt{2\epsilon}$  test will work when the test runs long enough. Of course, one strength of the  $\sqrt{2\epsilon}$  test is that it can sometimes detect unusual states, even when  $n$  is far too small to mix the chain, which is almost certainly the case for the application to gerrymandering later. When these short- $n$  runs are successful at detecting unusual states is, of course, dependent on the relationship of the presented state  $\sigma_0$  and its local neighborhood in the chain. An example is the random walk on the circle.

## 22.8. Application to Political Districting

Pennsylvania has 18 Congressional districts. According to the “one person, one vote” principle, Congressional districts are required by law to be roughly equal in population. Pennsylvania is divided into roughly 9,000 voting precincts. Say a division of these precincts into 18 districts to be a *valid districting* of Pennsylvania if each district differs in population from uniform equality by less than 2%, are contiguous, are simply connected (districts do not contain holes), and are “compact”. Roughly, this last condition prohibits districts with extremely contorted structure. The state space of the Markov chain is the set of valid districtings of Pennsylvania. One step of the Markov chain consists of randomly swapping a precinct on the boundary of a district to a neighboring district if the result is still a valid districting. Modify the chain to ensure the uniform distribution on valid districting is indeed the stationary distribution for the chain, see [CFP17b] for details. Observe that this Markov chain has a potentially huge state space; if the only constraint on valid districting was that the districts have roughly equal population, there would be  $10^{10000}$  or so valid districtings. (See the exercises for a justification of this estimate.) Although contiguity and especially compactness are severe restrictions that will decrease this number substantially, it seems difficult to compute effective upper bounds on the number of resulting valid districtings, and certainly, the number of valid districtings is still enormous. Impressively, these considerations are all immaterial to the general method of significance testing. Regarding mixing time, even in chains with relatively weak constraints on the districtings (and fast running time in implementation), the chains seem to mix too slowly to sample  $\pi$ , even heuristically.

Applying the  $\sqrt{2\epsilon}$  test involves the choice of a value function  $v(\sigma)$ , which assigns a real number to each districting. Two useful value functions are

- $v_{\text{var}}$  is the (negative) variance of the vector with the proportion of Democrats in each district of the districting (measured by quadrennial presidential votes), and
- $v_{\text{MM}}$  is the difference between the median and mean of the proportions of Democrats in each district.

The variance can change quickly with small changes in districtings, making it a sensitive value function. The median-mean difference  $v_{\text{MM}}$  metric has a long history in gerrymandering analysis. An important point is that these value functions are not based on an assumption that small values of  $v_{\text{var}}$  or  $v_{\text{MM}}$  directly imply gerrymandering. Instead, because the  $\sqrt{2\epsilon}$  test is valid for any fixed value function, these values are tools used to show statistical significance. Use these value functions because they are simple and natural functions on vectors that can be quickly computed, seem likely to be different for typical versus gerrymandered districtings, and have the potential to change relatively quickly with small changes in districtings. For chains of length  $2^{40}$  steps with various notions of valid districtings differing in compactness measure and threshold, the  $\sqrt{2\epsilon}$  test showed significance in the range from  $10^{-4}$  to  $10^{-5}$  for the  $v_{\text{MM}}$  value function and the range from  $10^{-4}$  to  $10^{-7}$  for the  $v_{\text{var}}$  value function, see [CFP17b].

It should also be kept in mind that, although the  $\sqrt{2\epsilon}$  Test gives a method to show the districting is unusual among districtings distributed according to the

stationary distribution  $\pi$ , it does so without giving a method to sample from the stationary distribution. In particular, the method cannot answer the question of how many seats Republicans and Democrats should have in a *typical* districting of Pennsylvania, because the chain is not selecting from the stationary distribution. Instead, the  $\sqrt{2\epsilon}$  gives a way to *disprove* the null hypothesis that a given districting is *not unusual* without sampling  $\pi$ . Consider the following specialization of the Outlier Test Algorithm for the political districting of a state:

- (1) Begin with the districting being evaluated.
- (2) Make a sequence of random changes to the districting, while preserving some set of constraints imposed on the districtings.
- (3) Evaluate the partisan properties of each districting encountered by simulating elections using past voting data and measuring  $v_{\text{var}}$  or  $v_{\text{MM}}$ .
- (4) Call the original districting “carefully crafted” or “gerrymandered” if the overwhelming majority of districtings produced by making small random changes are less partisan than the original districting.

Naturally, the test described above can be implemented so it precisely satisfies the hypotheses of the Theorems in this section. For this purpose, a (very large) set of comparison districtings are defined, to which the districting being evaluated belongs. For example, the comparison districtings may be the districtings built out of precincts (or some other unit) which are contiguous, equal in population up to some specified deviation, or include other constraints. A Markov chain  $X$  randomly walks through the districtings, where transitions in the chain correspond to changes in districtings. For example, a transition may correspond to randomly changing the district assignment of a randomly chosen Census Block which currently borders more than one district, subject to the constraints imposed on the comparison set. This is called a “flip chain” on the state space of all feasible districting. Alternatively, a “ReCom chain” method works as follows: merge two districts in the plan, generate a minimum spanning tree for the precincts in the merged district, then “split” the merged district into two new districts by finding a population-balanced cut of the minimum spanning tree. The “random changes” from Step 2 will then be precisely governed by the transition probabilities of the Markov chain  $X$ . By designing  $X$  so the uniform distribution  $\pi$  on the set of possible districtings  $\mathcal{X}$  is the stationary distribution for  $X$ , Theorem 22.16 gives an upper bound on the false positive, i.e. Type I error, probability for the null hypothesis of “not gerrymandered” declaration made in Step 4.

## 22.9. Chapter Ending Answer

Making a Type I error would be to do the statistical test, and *reject* the null hypothesis that the state is “not unusual” with respect to some function valuing the states when in fact, the state *is* typical with respect to the valuing. That is, to conclude the state is unusual when in fact it is typical.

Making a Type II error would be to do the statistical test, and *not reject* the null hypothesis that the state is “not unusual” with respect to some function valuing

the states when in fact, the state *is* unusual with respect to the valuing. That is, to conclude that the state is typical when in fact it is unusual.

## 22.10. Chapter Summary

### Key Concepts.

- (1) The  $\sqrt{2\epsilon}$  test is: Observe a trajectory  $X_0, X_1, X_2, \dots, X_n$  from the state  $X_0 \sim \pi$  for any fixed  $n$ . The event  $v(X_0)$  is an  $\epsilon$ -outlier among  $v(X_0), \dots, v(X_n)$  occurs with probability  $p$  which is at most  $\sqrt{2\epsilon}$ .
- (2)

**Theorem 22.29.** (a) Let  $X$  be a reversible Markov chain on  $\mathcal{X}$ .

(b) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(c) Given  $X_0$ , suppose for a random state  $x \sim \pi$ ,

$$\mathbb{P}[v(X) \leq v(X_0)] \leq \epsilon.$$

Then with probability  $p$  at least

$$\rho \geq 1 - \left(1 + \frac{\epsilon}{10\tau_{rel}}\right) \cdot \frac{1}{\sqrt{\pi_{min}}} \cdot \exp\left(\frac{-\epsilon^2 \cdot n}{20\tau_{rel}}\right)$$

$v(x)$  is a  $2\epsilon$ -outlier among  $v(X_0), v(X_1), \dots, v(X_n)$  where  $X_0, X_1, \dots, X_n$  is a random trajectory starting from  $X_0$ .

### Vocabulary.

- (1) A **value function** or *label* is a function  $v : \mathcal{X} \rightarrow \mathbb{R}$ . The value function has auxiliary information about the states of the chain and has no relationship to the transition probabilities of the Markov chain.
- (2) A real number  $\alpha_0$  is an  $\epsilon$ -**outlier** among  $\alpha_0, \alpha_1, \dots, \alpha_n$  if there are, at most,  $\epsilon(n+1)$  indices  $i$  for which  $\alpha_i \leq \alpha_0$ , in other words

$$\text{card}(\{\nu : \alpha_\nu \leq \alpha_0\}) \leq \epsilon(n+1).$$

- (3) For  $1 \leq \ell \leq n+1$  say  $\alpha_j$  is **among- $\ell$ -smallest** in  $\alpha_0, \dots, \alpha_n$  if there are at most  $\ell$  indices from  $0, \dots, n$  such that the value of  $\alpha_i$  is at most the value of  $\alpha_j$ . That is,  $\alpha_j$  is among- $\ell$ -smallest in  $\alpha_0, \dots, \alpha_n$  if  $\text{card}(\{\nu : \alpha_\nu \leq \alpha_j\}) \leq \ell$ . In particular,  $\alpha_j$  is among-1-smallest in  $\alpha_0, \dots, \alpha_n$  when its value is the unique minimum value.

### Notation.

- (1)  $X, X_0, X_n$  – Markov chain, starting state, general step of the chain.
- (2)  $\mathcal{X}$  – State space of a Markov chain
- (3)  $v : \mathcal{X} \rightarrow \mathbb{R}$  – value or label function
- (4)  $\pi$  – stationary distribution
- (5)  $x_0$  – a given state from the state space
- (6)  $\alpha_0, \alpha_1, \dots, \alpha_n$  – arbitrary real numbers for the definition of outliers
- (7)  $\epsilon$  – small real number

(8)

$$\rho(j; \ell, n) = \mathbb{P}[X_j \text{ is among-}\ell\text{-smallest in } X_0, \dots, X_n]$$

- (9)  $\rho(j; 0, n \mid \sigma)$  – the probability  $X_j = \sigma$  has the unique minimum value in the Markov chain of length  $n$  given the Markov passes through  $\sigma$  at step  $j$ .
- (10)  $\xi_j$  – the indicator variable that is 1 whenever  $X_j$  is among- $2\ell$ -smallest in  $X_0, \dots, X_n$
- (11)  $p_i^n$  – the probability in a  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_n$ , the minimum  $v$  label value occurs at  $X_i$ .
- (12)  $N$  – a large integer
- (13)  $\zeta_\nu = \pm 1$  – Bernoulli random variable with equal probability  $\frac{1}{2}$
- (14)  $\tau_{\text{rel}}$  – the relaxation time for  $X$  is  $1/(1 - \lambda_2)$
- (15)  $U$  – uniform distribution on a set

### 22.11. Sources

This section is adapted from [CFMP20, CFP17a, CFP19].

The first paragraph of the remark following Proposition 22.12 about Markov chains with distinct irreducible components is adapted from <https://math.stackexchange.com/questions/1636992/example-of-a-reversible-but-reducible-markov-chain>

The statement of Gillman’s Chernoff-Type Bound is modified from [Gil98, Theorem 2.1].

The remark about relaxation times and mixing times is adapted from [LPW09] and <https://math.stackexchange.com/questions/1382222/relaxation-time-and-mixing-time-of-markov-chains>

## 22.12. Algorithms and Scripts

**Input** : Number of balls  $N$  and probability of urn switch,  $p$   
**Output**: Table of empirical probabilities of  $\epsilon$ -Outlier Test success.

```

1  $N \leftarrow 7, p \leftarrow 1/2, q \leftarrow 1 - p$ 
  // Build  $(N + 1) \times (N + 1)$  transition probability matrix
2  $P_{11} \leftarrow q, P_{12} \leftarrow p$ 
3  $P_{N+1,N} \leftarrow q, P_{N+1,N+1} \leftarrow p$ 
4 for  $r \leftarrow 2$  to  $N$  do
5    $P_{r,r-1} \leftarrow (r - 1)/N \cdot q$ 
6    $P_{r,r} \leftarrow (N - (r - 1))/N \cdot q + (r - 1)/N \cdot p$ 
7    $P_{r,r+1} \leftarrow (N - (r - 1))/N \cdot p$ 
8 end
  // initialize and build Markov chain
9  $X_0 \leftarrow 0$ 
10 Build Markov chain object
11 Set pathLength array, nTrials array,  $\epsilon$ , initialize results
Algorithm. 12 foreach element in pathLength do
13   foreach element in nTrials do
14     outlierThreshold  $\leftarrow \text{floor}((\epsilon \cdot \text{pathLength} + 1)) + 1$ 
15     Initialize nEpsilonOutlier  $\leftarrow 0$ 
16     foreach  $i \leftarrow 1$  to nTrials do
17       Run Markov chain of length pathLength
18       Prepend initial state  $X_0$ 
19       if  $X_0 < \text{outlierThreshold}$  then
20         | increment nEpsilonOutlier
21       end
22     end
23     probEpsOutlier  $\leftarrow \text{nEpsilonOutlier} / \text{nTrials}$ 
24     Update results table with probEpsOutlier
25   end
26 end
27 Report results table

```

### Scripts.

**R:** R script for alternative Erhenfest outliers.

```

1 library(markovchain)
2
3 N <- 51; p <- 1/2; q <- 1 - p;
4 stateNames <- as.character( 0:N )
5 ## Be careful here, because states numbered from 0,
6 ## but R indexes from 1
7 transMatrix <- matrix(0, N+1,N+1)
8 transMatrix[1,1] <- q

```



```

9 transMatrix[1,2] <- p
10 transMatrix[N+1, N ] <- q
11 transMatrix[N+1, N+1] <- p
12 for (row in 2:N) {
13   transMatrix[row, row-1] <- ((row-1)/N)*q
14   transMatrix[row,row] <- ((N-(row-1))/N)*q + ((row
-1)/N)*p
15   transMatrix[row,row+1] <- ((N-(row-1))/N)*p
16 }
17
18 startState <- "0"
19
20 altEhernfest <- new("markovchain", transitionMatrix=
  transMatrix,
21                      states=stateNames, name="
  AltEhernfest")
22
23 pathLength <- c(199, 399, 599, 999)
24 nTrials <- c(200, 400, 800, 1600)
25
26 eps <- 0.01
27
28 results <- matrix(0, length(pathLength), length(
  nTrials))
29
30 for (pL in 1:length(pathLength)) {
31   for (nT in 1:length(nTrials)) {
32
33     outlierThreshold <- floor( eps * (pathLength[pL] + 1)
      ) + 1
34
35     nEpsOutlier<- 0
36
37     for (i in 1:nTrials[nT]) {
38
39       path <- rmarkovchain(n=pathLength[pL],
40                           object = altEhernfest,
41                           t0 = startState)
42       fullPath <- c(startState, path)
43       labelFullPath <- as.numeric(fullPath)
44       labelStartState <- as.numeric(startState)
45       if (!identical(sort(labelFullPath)[
outlierThreshold], labelStartState)) {
46         nEpsOutlier <- nEpsOutlier + 1
47       }
48     }
49

```

```

50 probEpsOutlier <- nEpsOutlier/nTrials[nT]
51
52 results[pL, nT] <- probEpsOutlier
53 }
54 }
55
56 results

```

### 22.13. Problems to Work for Understanding

- 1: Compare the notion of  $\frac{1}{2}$ -outlier of a set of  $n+1$  real numbers  $\{\alpha_0, \alpha_1, \dots, \alpha_n\}$  to the median of the set.
- 2: For a set of real values  $\{\alpha_0, \dots, \alpha_n\}$ , compare the definition of “ $\epsilon$ -outlier” and “among- $\ell$ -smallest” to the notions of the rank of an element in the set and the rank of elements of a set.
- 3: Given a set of  $n+1$  real values  $\{\alpha_0, \dots, \alpha_n\}$ , show that  $\alpha_0$  is an  $\epsilon$ -outlier if and only if  $\alpha_0 < \alpha_{(t+1)}$  where  $t = \lfloor \epsilon(n+1) \rfloor$  is the “ $\epsilon$ -outlier threshold” and  $\alpha_{(0)}, \alpha_{(1)}, \dots, \alpha_{(n)}$  is the set sorted into increasing order.
- 4: Using Table 22.1, explain how the values  $[5, 3]$ ,  $[10, 7]$ , and  $[n, 11]$  in Table 22.2 are obtained.
- 5: Given a Markov chain  $X$  with value function  $v : \mathcal{X} \rightarrow \mathbb{R}$  and stationary distribution  $\pi$ , define for each  $j, \ell \leq n$  a real number  $\rho(j; \ell, n)$  which is the probability that for a  $\pi$ -stationary trajectory  $X_1, X_2, \dots, X_n$  the value  $v(X_j)$  is among- $\ell$ -smallest in  $v(X_1), v(X_2), \dots, v(X_n)$ . Show  $\rho(j; \ell, n)$  is well-defined.
- 6: Use the script to find the proportion of trials for which the state 0 is an 0.01-outlier for the alternative Ehrenfest urn model with  $N = 7, 21, 51$  balls and path length of the chain 199, 399, 599, 999 steps when executing 200, 400, 800 and 1600 trials. Display the results in three charts, one for each  $N$ .
- 7: Consider the bathroom occupancy example in the section on Stationary Distributions. That Markov chain is irreducible and aperiodic. Because the chain is formulated as a random walk on a weighted graph, it is reversible. Let the states be valued as “OOO”= 1, “OOV”= 2, “OFO”= 3, “OCO”= 4, “VO”= 5, “VV”= 6, so the greater value is a more desirable state. Using  $\epsilon = 0.1$  and a path length of 1000 steps starting from “OOO”, is the least desirable state “OOO” unusual with respect to this value function in the sense of being an  $\epsilon$ -outlier?

The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & 1/2 \\ 0 & 1/2 & 0 & 0 & 1/4 & 1/4 \\ 0 & 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ 1/6 & 1/6 & 1/6 & 0 & 1/2 & 0 \\ 1/6 & 1/6 & 0 & 1/6 & 0 & 1/2 \end{pmatrix} \end{matrix}.$$

8: Pennsylvania is divided into roughly 9,000 precincts. Define a division of these precincts into 18 congressional districts to be a valid districting of Pennsylvania if districts are equal in population. For purposes of the problem, assume precincts are approximately equal in population. (This is not a valid assumption, precincts can have widely varying populations between rural and urban areas.) Also assume the only constraint on a valid districting is the districts have roughly equal population. (This is not the only constraint, districts are also required to be connected and to be compact, that is, have no extremely contorted shapes.) Justify the claim that there would be  $10^{10000}$  or so valid districtings under this simple assumption.

9: Cite a reference to a theorem from classical probability for the probability an  $n$ -step 1-dimensional random walk from  $X_0$  takes a first step to the right and does not return to the origin.

10: Verify

$$\frac{1}{2^{n+1}} \binom{n}{n/2} \sim \frac{1}{\sqrt{2\pi n}}.$$

## Parallel Chain Significance Testing

A 1989 paper of Besag and Clifford [BC89] described a more sensitive test related to the  $\sqrt{2\epsilon}$  test to bound the probability that a state from a Markov chain is unusual. This section derives the Besag-Clifford Test and even more sensitive statistical tests to detect that a given state from a stationary distribution of a reversible Markov chain is unusual. These tests based on parallel Markov chains can efficiently separate the probability of being unusual from the size of the effect. The separation simplifies the interpretation of these tests.

The *research hypothesis* is again:

The given state is unusual with respect to some value measure.

The *null hypothesis* is again:

The given state is not unusual with respect to some value measure.

Mathematicians Only: prolonged scenes of intense rigor.

### 23.1. Chapter Starter Question

For what positive values of  $\epsilon$  is  $\epsilon < 2\epsilon < \sqrt{2\epsilon}$ ? For purposes of this section, for what values of  $\epsilon$  is the “Besag-Clifford Test” better than the “Parallel  $2\epsilon$  Test”, which in turn is more discriminating than the “Serial  $\sqrt{2\epsilon}$  Test”?

### 23.2. Two Chain Significance Tests

Recall the definitions

$$\rho(j; \ell, n) = \mathbb{P}[v(X_j) \text{ is among-}\ell\text{-smallest in } v(X_0), \dots, v(X_n)]$$

and

$$\rho(j; \ell, n \mid \sigma) = \mathbb{P}[v(X_j) \text{ is among-}\ell\text{-smallest in } v(X_0), \dots, v(X_n) \mid X_0 = \sigma]$$

for  $0 \leq j, \ell \leq n$ . With a slight change in the parameter notation, define the  $n+1$ -vector

$$(\rho(0; \epsilon, n), \rho(1; \epsilon, n), \dots, \rho(n; \epsilon, n))$$

where for each  $i$ ,  $\rho(i; \epsilon, n)$  is the probability that in a  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_n$ ,  $v(X_i)$  is among the smallest  $\epsilon$ -fraction of indices in the list  $v(X_0), v(X_1), \dots, v(X_n)$ . Define  $\rho(0; \epsilon, k \mid \sigma_0)$  as the probability that on a trajectory  $\sigma_0 = X_0, X_1, \dots, X_n$ ,  $v(\sigma_0)$  is among the smallest  $\epsilon$ -fraction of values in the list  $v(X_0), v(X_1), \dots, v(X_k)$ . The goal of the next theorem is to get an improved bound on these probabilities using parallel Markov chains. First comes a simple lemma showing that joining two independent, reversible, and stationary chains still has the stationary distribution.

**Lemma 23.1.** (1) Let  $X$  be a reversible Markov chain with stationary distribution  $\pi$ .

(2) Let  $Y_0, Y_1, \dots, Y_n$  and  $Z_0, Z_1, \dots, Z_n$  be 2 independent trajectories of length  $n$  from  $X$  from a common starting point  $Y_0 = Z_0 = \sigma_0$ .

(3) Suppose  $\sigma_0 \sim \pi$ .

Then

$$Y_n, Y_{n-1}, \dots, Y_1, \sigma_0, Z_1, Z_2, \dots, Z_n$$

is a  $\pi$ -stationary trajectory.

**Proof.** (1) Stationarity implies

$$(Z_0, Z_1, \dots, Z_n) \sim (X_n, X_{n+1}, \dots, X_{2n}).$$

(2) Stationarity and reversibility imply

$$(Y_n, Y_{n-1}, \dots, Y_1, Y_0) \sim (X_0, X_1, \dots, X_n).$$

(3) The assumption that  $Y_1, Y_2, \dots$  and  $Z_1, Z_2, \dots$  are independent Markov chain trajectories from  $\sigma_0$  is equivalent to the condition

$$\begin{aligned} \mathbb{P}[Z_j = z_j \mid Z_{j-1} = z_{j-1}, \dots, Z_1 = z_1, Z_0 = Y_0 = \sigma_0, Y_1 = y_1, \dots, Y_n = y_n] \\ = \mathbb{P}[Z_j = z_j \mid Z_{j-1} = z_{j-1}, \dots, Z_1 = z_1, Z_0 = \sigma_0] \\ = \mathbb{P}[Z_j = z_j \mid Z_{j-1} = z_{j-1}] \\ = \mathbb{P}[X_{n+j} = z_j \mid X_{n+j-1} = z_{j-1}]. \end{aligned}$$

(4) By induction on  $j \geq 1$ , using step 2 as the base case and step 3 as the induction step,

$$(Y_n, Y_{n-1}, \dots, Y_0 = Z_0, Z_1, \dots, Z_j) \sim (X_0, X_1, \dots, X_n, X_{n+1}, \dots, X_{n+j}).$$

(5) Using  $j = n$  and  $Y_0 = Z_0 = \sigma_0$ ,

$$(Y_n, Y_{n-1}, \dots, \sigma_0, Z_1, \dots, Z_n) \sim (X_0, X_1, \dots, X_n, X_{n+1}, \dots, X_{2n}).$$

□

Recall, a real number  $\alpha_0$  is an  $\epsilon$ -outlier among  $\alpha_0, \dots, \alpha_n$  if

$$\text{card}(\{\nu : \alpha_\nu \leq \alpha_0\}) \leq \epsilon \cdot (n+1).$$

**Theorem 23.2** (Parallel  $2\epsilon$  Test). (1) Let  $X$  be a reversible Markov chain with stationary distribution  $\pi$ .

- (2) Let  $Y_0, Y_1, \dots, Y_n$  and  $Z_0, Z_1, \dots, Z_n$  be 2 independent trajectories of length  $n$  from  $X$  from a common starting point  $Y_0 = Z_0 = \sigma_0$ .
- (3) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.
- (4) Suppose  $\sigma_0 \sim \pi$ .
- Then for any  $n$

$$\mathbb{P}[v(\sigma_0) \text{ is an } \epsilon\text{-outlier among } v(\sigma_0), v(Y_0), v(Y_1), \dots, v(Y_n), v(Z_1), \dots, v(Z_n)] < 2\epsilon.$$

**Proof.** (1) Given a Markov chain  $X$  with values  $v : \mathcal{X} \rightarrow \mathbb{R}$  and stationary distribution  $\pi$ , define for each  $j, \ell \leq n$  the probability  $\rho(j; \ell, n)$  that for a  $\pi$ -stationary trajectory  $X_1, X_2, \dots, X_n$  the value  $v(X_j)$  is among- $\ell$ -smallest in  $v(X_1), v(X_2), \dots, v(X_n)$ . All  $\pi$ -stationary trajectories  $X_1, X_2, \dots, X_n$  of fixed length  $n$  are all identical in distribution so  $\rho(j; \ell, n)$  is well-defined. (See the exercises in the previous section.)

- (2) If the sequence  $X_1, X_2, \dots, X_n$  is a  $\pi$ -stationary trajectory for  $X$ , then  $(X_{n-j}, \dots, X_n, \dots, X_{2n-j})$  is an identically distributed sequence. Thus the probability that  $v(X_n)$  is among- $\ell$ -smallest in

$$v(X_{n-j}), \dots, v(X_n), \dots, v(X_{2n-j})$$

is  $\rho(j; \ell, n)$ .

- (3) Observe that the event

$$[v(X_n) \text{ is among-}\ell\text{-smallest in } v(X_{n-j}), \dots, v(X_n), \dots, v(X_{2n-j})]$$

occurs if the event

$$[v(X_n) \text{ is among-}\ell\text{-smallest in } v(X_0), \dots, v(X_n), \dots, v(X_{2n})]$$

occurs, for all  $j = 0, \dots, n$ . It follows that  $\rho(n; \ell, 2n) \leq \rho(j; \ell, n)$ .

- (4) By 3,

$$(n+1)\rho(n; \ell, 2n) \leq \sum_{\nu=0}^n \rho(\nu; \ell, n).$$

- (5) Let  $\mathbf{1}_j$  be the indicator variable that is 1 whenever  $X_j$  is among- $\ell$ -smallest among  $X_0, \dots, X_n$ . The sum  $\sum_{\nu=0}^n \rho(\nu; \ell, n) = \mathbb{E}[\sum_{\nu=0}^n \mathbf{1}_\nu]$  is the expected number of indices  $j \in \{0, \dots, n\}$  such that  $v(X_j)$  is among- $\ell$ -smallest from  $v(X_0), \dots, v(X_n)$ , so

$$(23.1) \quad \sum_{\nu=0}^n \rho(\nu; \ell, n) \leq \ell.$$

(The proof of the next theorem also uses this inequality.)

- (6) Then

$$\rho(n; \ell, 2n) = \frac{1}{n+1} \sum_{\nu=0}^n \rho(\nu; \ell, n) \leq \frac{\ell}{n+1} < 2 \cdot \frac{\ell}{2n+1}.$$

- (7) As in the section on Serial Significance, use the slight abuse of notation that  $\rho(i; \epsilon, n)$  is the probability that in a  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_n$ ,  $v(X_i)$  is among  $\lfloor \epsilon(n+1) \rfloor$ -smallest in  $v(X_0), v(X_1), \dots, v(X_n)$ .
- (8) Then

$$\rho(n; \epsilon, 2n) \leq 2 \frac{\lfloor \epsilon(2n+1) \rfloor}{2n+1} \leq 2 \frac{\epsilon(2n+1)}{2n+1} = 2\epsilon.$$

□

**Remark 23.3.** The remaining theoretical question is the largest possible value of  $\rho(n; \epsilon, 2n)$  as a function of  $\epsilon$ .

**Remark 23.4.** Using Markov chains is an inherently serial process, each step follows from the previous step. However, as the name suggests, Theorem 23.23 creates the opportunity to use parallel computing to increase the ability to detect outliers. Later Theorems will expand testing to multiple chains.

**Example 23.5.** Consider a specific simple case of the alternative Ehrenfest urn model. The setup of the urn model is repeated for convenient reference. Two urns, labeled  $A$  and  $B$ , contain a total of  $N = 7$  balls. At each step a ball is selected at random with all selections equally likely. Then an urn is selected, urn  $A$  with probability  $p = \frac{1}{2}$  and urn  $B$  with probability  $q = 1 - p = \frac{1}{2}$  and the ball is moved to that urn. The state at each step is the number of balls in the urn  $A$ , from 0 to  $N$ . Start from a random state chosen from the binomial distribution, which is the stationary distribution for this chain. All states are accessible and all states communicate, so the chain is irreducible. All states are recurrent with no transient states. The chain is periodic with period 1, so it is regular. The standard Ehrenfest urn model, without the random choice of urns at each step, is periodic with period 2. Having period 1 makes interpretation of the results simpler.

For this simple example, let the value function be the number of balls in urn  $A$ , so that the value function is identical with the state number. The simplicity of the alternative Ehrenfest urn model limits the possibilities for value functions.

This example uses the reproducible simulation of the alternate Ehrenfest urn model in `simParRhoProb.R`. The path length, or number of steps, is 10, short enough to be comprehensible, long enough have some content. Including the start state, the Markov chain has 11 values. The number of trials is 15, enough to illustrate the variety of sample paths, but not too many to overwhelm.

For each trial, first the simulation generates a chain of length 11 and the values along the paths are recorded in the rows of an  $15 \times 11$  matrix. Then for each given step  $j$  along the path, the count of other step values along the path less than or equal to the given step value is compared to  $\ell$ . If the count is less than or equal to  $\ell$ , that makes the given step value at  $j$  among  $\ell$ -smallest and the count in a  $11 \times 11$  matrix is incremented. When done, divide the counting matrix by the number of trials, 15, to give an empirical estimate of  $\rho(j; 0, n)$ . This is just as in the example in the section on Serial Significance. Summing down each column gives the values in Table 23.1. The table illustrates the inequality  $\sum_{\nu=0}^n \rho(\nu; \ell, n) \leq \ell + 1$  in step 4 in the proof of the Parallel  $2\epsilon$  Test.

For each trial, next the simulation generates two independent chains of length 11 starting from the first state. One chain with the common starting value is

$\ell$	1	2	3	4	5	6
$\sum_{\nu=0}^n \rho(\nu; \ell, n)$	0.267	0.667	1.733	2.600	3.067	3.467
$\ell$	7	8	9	10	11	
$\sum_{\nu=0}^n \rho(\nu; \ell, n)$	4.133	4.933	7.933	8.933	11.000	

**Table 23.1.** Empirical values of  $\sum_{\nu=0}^n \rho(\nu; \ell, n)$  to illustrate the inequality (4) in the proof of Theorem 23.23

reversed and concatenated with the second chain and the values along the paths are recorded in the rows of a  $15 \times 21$  matrix. This creates trials for paths as in Lemma 23.1. For the starting step value (the 11th along the concatenated path), the count of other step values along the path less than or equal to the starting step value is compared to  $\ell$ . If the count is less than or equal to  $\ell$ , that makes the given step value at 11 among- $\ell$ -smallest and the count in an 11 vector is incremented. When done, divide the vector by the number of trials, 15, to give an empirical estimate of  $\rho(n; \ell, 2n)$  as in step 3 of the proof. Comparing the empirical probabilities illustrates  $\rho(n; \ell, 2n) \leq \rho(j; \ell, n)$  with this simulation.

Finally, for  $\epsilon = 0.1$ , the empirical probability of the starting value being an  $\epsilon$ -outlier among the values from the concatenated path is less than  $\epsilon$ .  $\nabla$

**Theorem 23.6** (Besag-Clifford Test). (1) Let  $X$  be a reversible Markov chain on  $\mathcal{X}$  with a stationary distribution  $\pi$ .  
(2) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a label function.  
(3) Fix a positive integer  $n$ .  
(4) Suppose  $\sigma_0 \sim \pi$ .  
(5) Integer  $\xi$  is chosen at random uniformly in  $\{0, \dots, n\}$ .  
(6) Let two independent trajectories  $Y_0, Y_1 \dots$  and  $Z_0, Z_1, \dots$  start from  $Y_0 = Z_0 = \sigma_0$ .

Then for any  $n$

$\mathbb{P}[v(\sigma_0) \text{ is an } \epsilon\text{-outlier among}$

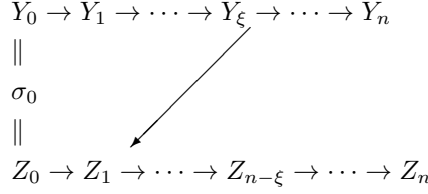
$$v(\sigma_0), v(Y_1), \dots, v(Y_\xi), v(Z_1), \dots, v(Z_{n-\xi})] \leq \epsilon.$$

**Remark 23.7.** See Figure 23.1 for a schematic diagram of the Besag-Clifford Test. Note that  $\sigma_0, Y_1, \dots, Y_\xi, Z_1, \dots, Z_{n-\xi}$  may not be a valid Markov chain. For instance, the transition  $Y_\xi$  to  $Z_1$  may not be an allowed transition. Since the Theorem only considers the probability of a set of values, failure to be a valid Markov chain sequence is not a problem.

**Proof of Theorem 23.24.** (1) The proof uses only equation (23.1).

- (2) Recall from the proof of Theorem 23.23 that the  $\rho(j; \ell, n)$  are fixed real numbers associated to a stationary Markov chain.
- (3) If  $\ell$  and  $n$  are fixed, and  $\xi$  is chosen at random uniformly from  $\{0, \dots, n\}$ , then the resulting  $\rho(\xi; \ell, n)$  is a random variable uniformly distributed on the set of real numbers  $\{\rho(0; \ell, n), \dots, \rho(n; \ell, n)\}$ .





**Figure 23.1.** Schematic diagram of the Besag-Clifford Test. The short wide-head arrows are the Markov chain transitions, the long narrow-head arrow represents the switch from the  $Y$  trajectory to the  $Z$  trajectory.

- (4) The probability that  $v(\sigma_0)$  is among- $\ell$ -smallest in

$$v(\sigma_0), v(Y_1), \dots, v(Y_\xi), v(Z_1), \dots, v(Z_{n-\xi})$$

is

$$\frac{1}{n+1}(\rho(0; \ell, n) + \rho(1; \ell, n) + \dots + \rho(n; \ell, n)) \leq \frac{\ell}{n+1}$$

using equation (23.1).

- (5) This observation uses a variant of Lemma 23.1 that for any  $j$ ,

$$Y_j, \dots, Y_1, \sigma_0, Z_1, \dots, Z_{n-j}$$

is a  $\pi$ -stationary trajectory.

□

**Remark 23.8.** Notice that  $\epsilon$  would be the correct value of the probability if, for example, the Markov chain is simply a collection of independent random uniform samples from  $[0, 1]$  with the identity as the value function. The values of the  $Y$  and  $Z$  trajectories would then be a collection of  $2n + 1$  random uniform samples from  $[0, 1]$  and the probability  $v(\sigma_0)$  is an  $\epsilon$ -outlier would be  $\epsilon$ .

The striking thing about Theorem 23.24 is that it has a better dependence on the parameter  $\epsilon$  than either the  $\sqrt{2\epsilon}$  Test or the Parallel  $2\epsilon$  Test. The sacrifice is in the theorem's more complicated intuitive interpretation.

In applications of these statistical tests to aspects of public policy such as the gerrymandering example in [CFMP20], it is desirable to have tests with simple, intuitive interpretations. To enable better significance testing in the policy domain, one goal of this section is to prove a theorem enabling Markov chain significance testing that is intuitively interpretable in the sense of Proposition 22.12 while having linear dependence on  $\epsilon$ , as in Theorem 23.24.

**Remark 23.9.** One common feature of the tests based on Proposition 22.12 and 23.24 is the use of randomness. In particular, the probability space underneath these theorems includes both the random choice of  $\sigma_0$  assumed by the null hypothesis and the random steps taken by the Markov chain from  $\sigma_0$ . Thus the measures of “how much (globally) unusual”  $\sigma_0$  is with respect to its performance in the local outlier test and “how sure” we are that  $\sigma_0$  is unusual in this respect are intertwined in the final  $p$ -value. In particular, the effect size and the statistical significance are not explicitly separated.

**Example 23.10.** Once again, consider a specific simple case of the alternative Ehrenfest urn model with  $N = 7$  balls. This example uses the reproducible simulation of the alternate Ehrenfest urn model in `simBesagClifford.R`. The path length, or number of steps, is 10, short enough to be comprehensible, long enough have some content. Including the start state, the Markov chain has 11 values. The number of trials is 15, enough to illustrate the variety of sample paths, but not too many to overwhelm.

For each trial, the simulation generates two independent chains of length 11 starting from the common starting state. Choosing integer  $\xi$  at random uniformly in  $\{0, \dots, n\}$  the values  $v(\sigma_0), v(Y_1), \dots, v(Y_\xi), v(Z_1), \dots, v(Z_{n-\xi})$  are recorded in the rows of an  $15 \times 11$  matrix. This creates trials as in Theorem 23.24. Then for each starting step value along the concatenated path, the count of other step values along the path less than or equal to the starting step value is compared to  $\ell$ . If the count is less than or equal to  $\ell$ , that makes the starting step value among- $\ell$ -smallest and the count in an 11 vector is incremented. When done, divide the vector by the number of trials, 15, to give an empirical estimate of the probability of an outlier as in Theorem 23.24. Comparing the empirical probabilities illustrates the Besag-Clifford Test with this simulation.

Finally, for  $\epsilon = 0.1$ , the empirical probability of the starting value being an  $\epsilon$ -outlier among the values from the concatenated path is the empirical probability of being among-1-smallest, namely 0, which is less than  $\epsilon$ .

▽

### 23.3. The Multiple Chain Significance Test

Extend the slight abuse of notation adopted in the previous section. For each  $j$ , let  $\rho(j; \epsilon, n \mid \sigma)$  be the probability that in an  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_n$ ,  $v(X_i)$  is among- $\lfloor \epsilon(n+1) \rfloor$ -smallest in  $v(X_0), v(X_1), \dots, v(X_n)$  given that  $X_j = \sigma$ .

**Definition 23.11.** Let  $0 < \epsilon \ll 1$  and  $0 < \alpha \ll 1$ . For a fixed value of  $n$ , the state  $\sigma_0$  is an  $(\epsilon, \alpha)$ -outlier in  $\mathcal{X}$  if, among all states in  $\mathcal{X}$ ,  $\rho(0; \epsilon, n \mid \sigma_0)$  is in the fraction  $\alpha$  of the values of  $\rho(0; \epsilon, n \mid \sigma)$  over all states  $\sigma \in \mathcal{X}$ , weighted according to  $\pi$ . In particular, being an  $(\epsilon, \alpha)$ -outlier measures the likelihood of  $\sigma_0$  failing the local outlier test, ranked against all other states  $\sigma \sim \pi$  of the chain  $X$ . ◇

Whether  $\sigma_0$  is an  $(\epsilon, \alpha)$ -outlier is a deterministic question about the properties of  $\sigma_0$ ,  $X$ , and  $v$ . It is a deterministic measure (defined in terms of the Markov chain distribution) of the extent  $\sigma_0$  could be unusual in value compared to all of  $\mathcal{X}$ , keeping in mind the stationary distribution for the starting value.

**Example 23.12.** For another example, fix  $n = 10^9$ . If  $\sigma_0$  is a  $(10^{-6}, 10^{-5})$ -outlier for  $X$  and  $\pi$  is the uniform distribution, this means that among all states  $\sigma \in \mathcal{X}$ ,  $\sigma_0$  is more likely than all but a  $10^{-5}$ -fraction of states to have an  $v$ -value in the least  $10^{-6}$ -fraction of values  $v(X_0), v(X_1), \dots, v(X_{10^9})$ . The probability space underlying the “more likely” claim here just concerns the choice of the random trajectory  $X_1, \dots, X_{10^9}$  from  $X$ . ▽

State	0	1	2	3	4	5	6	7
$\pi$	0.467	0.333	0.267	0.067	0.000	0.000	0.000	0.000
	0.008	0.055	0.164	0.273	0.273	0.164	0.055	0.008
	0.004	0.018	0.044	0.018	0.000	0.000	0.000	0.000

**Table 23.2.** Empirical estimates of being an  $(\epsilon, \alpha)$  outlier for the small alternate Ehrenfest urn model. The second row is the rough probability of being a  $\epsilon$ -outlier ( $\epsilon = 0.1$ ) starting from the state in the top row, rounded to three places. The third row is the stable distribution  $\text{Bin}(7, 0.5)$  rounded to three places. The fourth row is the weighted approximation of being an  $\epsilon$ -outlier as a product of the second and third rows.

**Example 23.13.** Once again consider a specific simple case of the alternative Ehrenfest urn model with  $N = 7$  balls. This example uses the reproducible simulation of the alternate Ehrenfest urn model in `simEpsAlpha.R`. The path length, or number of steps, is  $n = 10$ , short enough to be comprehensible, long enough have some content. This is not long enough to converge to the stationary distribution, so the example is only explanatory. Including the start state, each simulation of the Markov chain has 11 values. For the example take  $\epsilon = 0.1$ , so the smallest fraction of values will be  $\lfloor \epsilon(n+1) \rfloor = \lfloor 0.1 \cdot 11 \rfloor = 1$  value. That is, the value under consideration must be the unique minimum of the set of chain values. For this example, in turn use each possible state as the starting state. The number of trials for each start state is 15, enough to illustrate the variety of sample paths, but not too many to overwhelm. Simulate the Markov chain from the start state for each trial and record the path. The record of paths will be a 3-dimensional array of size  $15 \times 11 \times 8$ . The array has 8 planes, one for each start state. Each plane has 15 rows for the trials, and the 11 columns are the step number, recording the state at that step for that trial. For each trial tally the number of states less than or equal to the start state. If that tally is less than or equal to 1, the start state is the unique minimum, and increment the count of “start state as unique minimum” from the trials. Dividing by the number of trials gives an approximation for the empirical probability (from the few trials in the simulation) of being an  $\epsilon$ -outlier *starting from that state*. According to the definition, the probability should be weighted according to  $\pi$ . Table 23.2 gives the empirical probability of being an  $\epsilon$ -outlier starting from the state and the probability of being an  $\epsilon$ -outlier weighted by the stationary distribution.

The rough fraction of chains starting from a random state from the stationary distribution and resulting in the starting state being an  $\epsilon$ -outlier is  $0.004 + 0.018 + 0.044 + 0.018 = 0.084$ . The rough fraction of chains starting from a random state from the stationary distribution other than 0 and resulting in the starting state being an  $\epsilon$ -outlier is  $0.018 + 0.044 + 0.018 = 0.080$ . This means that starting from a random state from the stationary distribution, 0 is more likely than all but about a 0.080-fraction of states to have an  $v$ -value in the least 0.1-fraction of values. Therefore, from this small and rough but comprehensible example, 0 is an  $(0.1, 0.08)$ -outlier.

▽

The following theorem is an analogue of Proposition 22.12. While tests based on Proposition 22.12 and Theorem 22.27 take as their null hypothesis that  $\sigma_0 \sim \pi$  is not unusual in the value function, the following Theorem 23.25 takes as its null hypothesis  $\sigma_0$  is not an  $(\epsilon, \alpha)$ -outlier.

Recall  $\rho(j; \epsilon, n \mid \sigma)$  is the probability that  $v(X_j)$  is in the lowest  $\epsilon$  fraction of the values  $v(X_0), \dots, v(X_n)$  conditioned on the event  $X_j = \sigma$ .

**Lemma 23.14.** *If  $\sigma_0$  is not an  $(\epsilon, \alpha)$ -outlier, then*

$$\rho(0; \epsilon, n \mid \sigma_0) \leq \sqrt{\frac{2\epsilon}{\alpha}}.$$

**Proof.** (1) Consider a  $\pi$ -stationary trajectory  $X_0, \dots, X_n, \dots, X_{2n}$  and condition on the event  $X_n = \sigma$  for some arbitrary  $\sigma \in \mathcal{X}$ . Since  $X$  is reversible, this trajectory is two independent trajectories,  $X_n, X_{n+1}, \dots, X_{2n}$  and  $X_n, X_{n-1}, X_{n-2}, \dots, X_0$  both beginning from  $\sigma$ .

(2) Let  $A$  and  $B$  be the events  $v(X_n)$  is an  $\epsilon$ -outlier among the lists  $v(X_0), \dots, v(X_n)$  and  $v(X_n), \dots, v(X_{2n})$ , respectively. The event  $A \cap B$  would have  $v(X_n)$  among the lowest  $\epsilon$  fraction of values in the long chain of  $2n$  steps. By the independence of the trajectories,

$$(23.2) \quad (\rho(0; \epsilon, n \mid \sigma))^2 = \mathbb{P}[A \cap B] \leq \rho(n; \epsilon, 2n \mid \sigma).$$

(3) The assumption that the given  $\sigma_0 \in \mathcal{X}$  is not an  $(\epsilon, \alpha)$ -outlier means that for a random  $\sigma \sim \pi$

$$(23.3) \quad \mathbb{P}[\rho(0; \epsilon, n \mid \sigma) \geq \rho(0; \epsilon, n \mid \sigma_0)] \geq \alpha.$$

(4) Equation (23.2) gives  $(\rho(0; \epsilon, n \mid \sigma))^2 \leq \rho(n; \epsilon, 2n \mid \sigma)$  while Theorem 23.23 gives  $\rho(n; \epsilon, 2n \mid \sigma) \leq 2\epsilon$ .

(5) Taking expectations with respect to a random  $\sigma \sim \pi$  gives

$$\begin{aligned} \mathbb{E}_{\sigma \sim \pi} [(\rho(0; \epsilon, n \mid \sigma))^2] &\leq \mathbb{E}_{\sigma \sim \pi} [\rho(n; \epsilon, 2n \mid \sigma)] \\ &= \rho(n; \epsilon, 2n) \leq 2\epsilon. \end{aligned}$$

(6) On the other hand, with (23.3)

$$\alpha \cdot (\rho(0; \epsilon, n \mid \sigma))^2 \leq \mathbb{E}_{\sigma \sim \pi} [(\rho(0; \epsilon, n \mid \sigma))^2]$$

so that

$$(\rho(0; \epsilon, n \mid \sigma))^2 \leq \frac{2\epsilon}{\alpha}.$$

□

**Theorem 23.15.** (1) *Let  $X$  be a reversible Markov chain with stationary distribution  $\pi$ .*

(2) *Let*

$$\begin{aligned} \mathbf{X}^1 &= (X_0^1, X_1^1, \dots, X_n^1) \\ &\vdots \\ \mathbf{X}^m &= (X_0^m, X_1^m, \dots, X_n^m) \end{aligned}$$

be  $m$  independent trajectories of length  $n$  from  $X$  starting from a common starting point  $X_0^1 = X_0^2 = \dots = X_0^m = \sigma_0$ .

- (3) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.
- (4) Define the random variable  $\mathcal{N}$  to be the number of trajectories  $\mathbf{X}^i$  on which  $\sigma_0$  is an  $\epsilon$ -outlier.
- (5) Suppose  $\sigma_0$  is not an  $(\epsilon, \alpha)$ -outlier.

Then

$$\mathbb{P} \left[ \mathcal{N} \geq m \sqrt{\frac{2\epsilon}{\alpha}} + r \right] \leq e^{-r^2/(2m\sqrt{2\epsilon/\alpha}+r)}.$$

**Proof.** (1) For a  $\pi$ -stationary trajectory the probability  $\rho(0; \epsilon, n \mid \sigma_0)$  is the probability that on a trajectory  $\sigma_0 = X_0, X_1, \dots, X_n$ ,  $v(\sigma_0)$  is among the smallest  $\epsilon$  fraction of values in the list  $v(X_0), v(X_1), \dots, v(X_n)$ .

- (2) The random variable  $\mathcal{N}$  is the number of trajectories  $X^i$  from  $\sigma_0$  on which  $\sigma_0$  is observed to be an  $\epsilon$ -outlier with respect to the valuing  $v$ . Using the Lemma, the random variable  $\mathcal{N}$  is the sum of  $m$  independent Bernoulli random variables with value 1 with probability less than  $\sqrt{\frac{2\epsilon}{\alpha}}$ .

- (3) Then  $\mathbb{E}[\mathcal{N}] \leq m \sqrt{\frac{2\epsilon}{\alpha}}$ . By Chernoff's bound (in the form

$$\mathbb{P}[X \geq (1 + \delta)\mu] \leq e^{-\delta^2 \mu / (2 + \delta)}$$

for a sum of Bernoulli random variables with mean  $\mu$ )

$$\mathbb{P} \left[ \mathcal{N} \geq (1 + \delta)m \sqrt{\frac{2\epsilon}{\alpha}} \right] \leq e^{-(\delta^2 m \sqrt{2\epsilon/\alpha}) / (2 + \delta)}.$$

- (4) Using  $\delta = r / (m \sqrt{2\epsilon/\alpha})$  and substituting gives

$$\mathbb{P} \left[ \mathcal{N} \geq m \sqrt{\frac{2\epsilon}{\alpha}} + r \right] \leq e^{-r^2/(2m\sqrt{2\epsilon/\alpha}+r)}.$$

□

**Remark 23.16.** When  $m$  is a reasonable size for calculation, it may make more sense to use the exact binomial tail in place of the Chernoff bound. That is the content of the following Corollaries.

**Corollary 23.17.** *Given the hypotheses in Theorem 23.25, then*

$$\mathbb{P}[\mathcal{N} \geq K] \leq \sum_{\nu=K}^m \binom{m}{\nu} \left( \sqrt{\frac{2\epsilon}{\alpha}} \right)^\nu \left( 1 - \sqrt{\frac{2\epsilon}{\alpha}} \right)^{m-\nu}.$$

**Corollary 23.18.** *Given the hypotheses of Theorem 23.25, then*

$$\mathbb{P}[\sigma_0 \text{ is an } \epsilon\text{-outlier on all of } \mathbf{X}^1, \dots, \mathbf{X}^m] \leq \left( \frac{2\epsilon}{\alpha} \right)^{m/2}.$$

### 23.4. The Improved Multiple Chain Significance Test

The following Theorem 23.26 is the analog of Theorem 23.25 using an analog of Besag and Clifford's Theorem 23.24 in place of Proposition ?? in the proof. This version pays the price of using a random  $n$  instead of a fixed  $n$  for the notion of an  $(\epsilon, \alpha)$ -outlier, but has the advantage that the constant 2 is eliminated from the bound. As in Theorem 23.25, the notion of  $(\epsilon, \alpha)$ -outlier here is still just defined with respect to a single path, although Theorem 23.24 depends on using two independent trajectories.

**Theorem 23.19.** (1) Let  $X$  be a reversible Markov chain.

(2) Let  $n_1, \dots, n_m$  be  $m$  integers independently drawn from a geometric distribution with mean  $\mu$  supported on  $0, 1, 2, \dots$

(3) Let

$$\begin{aligned} \mathbf{X}^1 &= (X_0^1, X_1^1, \dots, X_{n_1}^1) \\ &\vdots \\ \mathbf{X}^m &= (X_0^m, X_1^m, \dots, X_{n_m}^m) \end{aligned}$$

be  $m$  independent trajectories, each respectively of length  $n_i$ , from  $X$  starting from a common starting point  $X_0^1 = X_0^2 = \dots = X_0^m = \sigma_0$ .

(4) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(5) Define the random variable  $\mathcal{N}$  to be the number of trajectories  $\mathbf{X}^i$  with  $\sigma_0$  as an  $\epsilon$ -outlier.

(6) Suppose  $\sigma_0$  is not an  $(\epsilon, \alpha)$ -outlier.

Then

$$\mathbb{P} \left[ \mathcal{N} \geq m \sqrt{\frac{\epsilon}{\alpha}} + r \right] \leq e^{-r^2 / (2m \sqrt{\epsilon/\alpha} + r)}.$$

**Remark 23.20.** Observe carefully the difference in conclusions of this Theorem 23.26 from Theorem 23.25 is the absence of the factor 2 in the square root, so Theorem 23.26 is a slight improvement in the probability estimates. The improvement comes at the cost of a more complicated set of parallel Markov chains.

**Proof.** (1) For a  $\pi$ -stationary trajectory  $X_0, \dots, X_n$  and a real number  $\mu$ , as a modification of a previous notation define  $\rho(0; \epsilon, \mu \mid \sigma)$  to be the probability that  $v(X_j)$  is in the lowest  $\epsilon$  fraction of the values  $v(X_0), \dots, v(X_n)$ , conditioned on the event  $X_0 = \sigma$ , where the length  $n$  is chosen from a geometric distribution with mean  $\mu$  supported on  $\nu = 0, 1, 2, \dots$ . The modification substitutes the geometric distribution parameter  $\mu$  for the fixed trajectory length. Recall the definition of the geometric distribution with mean  $\mu$  supported on  $0, 1, 2, \dots$ :

$$\mathbb{P}[n = \nu] = \frac{1}{\mu + 1} \left( 1 - \frac{1}{\mu + 1} \right)^\nu.$$

- (2) It suffices to prove that if  $\sigma_0$  is not an  $(\epsilon, \sigma)$ -outlier with respect to  $n$  drawn from the geometric distribution with mean  $\mu$ , then

$$\rho(0; \epsilon, \mu \mid \sigma) \leq \sqrt{\frac{\epsilon}{\alpha}}.$$

Then the proof can proceed just as in Theorem 23.25.

- (3) To prove the previous assertion, suppose that  $n_1$  and  $n_2$  are independent geometrically distributed random variables with mean  $\mu$ , and consider a  $\pi$ -stationary trajectory  $X_0, \dots, X_{n_1}, \dots, X_{n_1+n_2}$  of random length  $n_1 + n_2$ , and condition on the event  $X_{n_1} = \sigma$  for some arbitrary  $\sigma \in \mathcal{X}$ . Since the Markov chain  $X$  is reversible, view this trajectory as two independent trajectories  $X_{n_1}, X_{n_1+1}, \dots, X_{n_1+n_2}$  and  $X_{n_1}, X_{n_1-1}, \dots, X_0$  both beginning from  $X_{n_1} = \sigma$ , of random lengths  $n_2$  and  $n_1$  respectively.
- (4) Letting  $A$  and  $B$  be the events  $v(X_{n_1})$  is an  $\epsilon$ -outlier among the lists  $v(X_0), \dots, v(X_{n_1})$  and  $v(X_{n_1}), \dots, v(X_{n_1+n_2})$  respectively,

$$\begin{aligned} \rho(0; \epsilon, \mu \mid \sigma)^2 &= \mathbb{P}[A \cap B] \leq \mathbb{P}[v(X_{n_1}) \text{ is an } \epsilon\text{-outlier among} \\ &\quad v(X_0), \dots, v(X_{n_1}), v(X_{n_1}), \dots, v(X_{n_1+n_2}) \mid X_{n_1} = \sigma]. \end{aligned}$$

Remember, in this last expression,  $n_1$  and  $n_2$  are random variables.

- (5) The assumption the given  $\sigma_0 \in \mathcal{X}$  is not an  $(\epsilon, \alpha)$ -outlier gives that for a random  $\sigma \sim \pi$ ,

$$\mathbb{P}[\rho(0; \epsilon, \mu \mid \sigma)] \geq \mathbb{P}[\rho(0; \epsilon, \mu \mid \sigma_0)] \geq \alpha.$$

- (6) Write

$$\begin{aligned} \alpha \cdot \rho(0; \epsilon, \mu \mid \sigma)^2 &\leq \mathbb{E}_{\sigma \sim \pi} [\rho(0; \epsilon, \mid \sigma)^2] \\ &\leq \mathbb{P}[v(X_{n_1}) \text{ is an } \epsilon\text{-outlier among} \\ &\quad v(X_0), \dots, v(X_{n_1}), v(X_{n_1}), \dots, v(X_{n_1+n_2})] \end{aligned}$$

where the last inequality follows from step 4.

- (7) Now a simple fact about geometric random variables, motivated by considering the right-hand side of step 6. Conditioning on the value for the length  $\ell = n_1 + n_2$  of the trajectory,  $n_1$  is uniformly distributed in the range  $0, \dots, \ell$ . This is ensured by the geometric distribution, simply because for any  $\ell$  and any  $x \in (0, \dots, \ell)$ , the probability

$$\begin{aligned} \mathbb{P}[n_1 = x \text{ and } n_2 = \ell - x] &= \left( \frac{1}{\mu + 1} \left( 1 - \frac{1}{\mu + 1} \right)^x \right) \cdot \left( \frac{1}{\mu + 1} \left( 1 - \frac{1}{\mu + 1} \right)^{\ell - x} \right) \\ &= \left( \frac{1}{\mu + 1} \right)^2 \left( 1 - \frac{1}{\mu + 1} \right)^\ell \end{aligned}$$

is independent of  $x$ .

- (8) In particular, conditioning on any particular value for the length  $\ell = n_1 + n_2$ , the probability  $v(X_{n_1})$  is an  $\epsilon$ -outlier on the trajectory is at most  $\epsilon$  since  $X_{n_1}$  is a uniformly randomly chosen element of the trajectory  $X_0, \dots, X_{n_1+n_2}$ .

This part of the proof is exactly the same as the proof of the Besag-Clifford Theorem.

(9) In particular, for the right hand side of the inequality in step 6

$$\begin{aligned} \alpha \cdot \rho(0; \epsilon, \mu | \sigma)^2 &\leq \mathbb{P}[v(X_{n_1}) \text{ is an } \epsilon\text{-outlier among} \\ &\quad v(X_0), \dots, v(X_{n_1}), v(X_{n_1}), \dots, v(X_{n_1+n_2})] \\ &\leq \max_i \mathbb{P}[v(X_{n_1}) \text{ is an } \epsilon\text{-outlier among} \\ &\quad v(X_0), \dots, v(X_{n_1}), v(X_{n_1}), \dots, v(X_{n_1+n_2}) \mid n_1 + n_2 = \ell] \leq \epsilon. \end{aligned}$$

This establishes the required inequality in step 2 and completes the proof.  $\square$

**Remark 23.21.** When  $m$  is not large, using the exact binomial tail in place of the Chernoff bound in (23.2) may be sensible. This gives the following Corollary.

**Corollary 23.22.** *Given the hypotheses of Theorem 23.26, then*

$$\mathbb{P}[\mathcal{N} \geq K] \leq \sum_{\nu=K}^m \binom{m}{\nu} \left( \sqrt{\frac{\epsilon}{\alpha}} \right)^k \left( 1 - \sqrt{\frac{\epsilon}{\alpha}} \right)^{m-k}.$$

More refined parallel test are discussed in [CFMP20], including an extension of the Besag-Clifford Test to multiple parallel chains, an extension to tree structures of Markov chains, and to state spaces with a product structure. The extensions are applied to examples of detecting claims of gerrymandering of political districts.

## 23.5. Multiple Testing Considerations

Theorem 23.25 uses  $m$  chains, each of which has a probability of having the starting state  $\sigma_0$  being an  $\epsilon$ -outlier where  $\epsilon$  is chosen small. For any one specific chain, the probability of erroneously rejecting the null hypothesis is small. However, the probability of *at least one* false report is much higher. Performing several tests, then allowing a significant result on any of them to be evidence for rejecting the hypothesis requires a multiple testing correction. Multiple testing, also called multiple comparisons, arises when a statistical analysis involves multiple simultaneous statistical tests, each having a potential to produce a “discovery”, on the same data set or dependent data sets. Specifically, there is a chance that the hypothesis which is actually true is rejected by the test, a Type I error. The error probability increases with multiple testing. A stated confidence level generally applies only to each test considered individually, but often it is desirable to have a confidence level for the whole family of simultaneous tests. Failure to compensate for multiple comparisons can have important consequences, see the exercises.

The wrong way to apply Theorem 23.25 directly with multiple Markov chains is the following. Run  $m$  trajectories, record the minimum  $\epsilon_i$  for which the starting state  $\sigma_0$  is an  $\epsilon_i$ -outlier on  $X^i$ . That is, the  $i$ th trajectory has  $j_i$  values  $v(X_{\nu_1}^i), \dots, v(X_{\nu_{j_i}}^i)$  less than or equal to  $v(\sigma_0)$ , so  $v(\sigma_0)$  is a  $\epsilon_i = \frac{j_i}{n}$ -outlier. This creates a list of outlier values  $\epsilon_1, \epsilon_2, \dots, \epsilon_m$ . Then post-hoc, freely choose the parameters  $\alpha$  and  $\epsilon$  in Theorem 23.25 to obtain some desired trade-off between  $\alpha$  and the  $p$ -value.



A solution is to set the parameter  $\epsilon \equiv \epsilon(t)$  as the  $t$ th-smallest element of the list  $\epsilon_1, \dots, \epsilon_m$  for some fixed value  $t$ . The case  $t = m$ , for example, corresponds to taking  $\epsilon$  as the maximum value, leading to the application of Corollary 23.18. More details and further discussion are in [CFMP20].

### 23.6. Chapter Ending Answer

For  $\epsilon > 0$ , always  $\epsilon < 2\epsilon$  so the “Besag-Clifford Test” is always more discriminating than the “Parallel  $2\epsilon$  Test”, which in turn is more discriminating than the “Serial  $\sqrt{2}\epsilon$  Test” for  $\epsilon < 1/2$ . Since  $\epsilon$  will usually be taken to be one of the traditional statistical significance values of  $p = 0.05$ ,  $p = 0.01$  or  $p = 0.001$ , the parallel tests will always be better.

### 23.7. Chapter Summary

#### Key Concepts.

(1)

**Theorem 23.23** (Parallel  $2\epsilon$  Test). (1) Let  $X$  be a reversible Markov chain with stationary distribution  $\pi$ .

(2) Let  $Y_0, Y_1, \dots, Y_n$  and  $Z_0, Z_1, \dots, Z_n$  be 2 independent trajectories of length  $n$  from  $X$  from a common starting point  $Y_0 = Z_0 = \sigma_0$ .

(3) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(4) Suppose  $\sigma_0 \sim \pi$ .

Then for any  $n$

$\mathbb{P}[v(\sigma_0) \text{ is an } \epsilon\text{-outlier among}$

$$v(\sigma_0), v(Y_1), \dots, v(Y_n), v(Z_1), \dots, v(Z_n)] < 2\epsilon.$$

(2)

**Theorem 23.24** (Besag-Clifford Test). (1) Let  $X$  be a reversible Markov chain on  $\mathcal{X}$  with a stationary distribution  $\pi$ .

(2) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a label function.

(3) Fix a positive integer  $n$ .

(4) Suppose  $\sigma_0 \sim \pi$ .

(5) Integer  $\xi$  is chosen uniformly in  $\{0, \dots, n\}$ .

(6) Let two independent trajectories  $Y_0, Y_1, \dots$  and  $Z_0, Z_1, \dots$  start from  $Y_0 = Z_0 = \sigma_0$ .

Then for any  $n$

$\mathbb{P}[v(\sigma_0) \text{ is an } \epsilon\text{-outlier among}$

$$v(\sigma_0), v(Y_1), \dots, v(Y_\xi), v(Z_1), \dots, v(Z_{n-\xi})] \leq \epsilon.$$

(3)

**Theorem 23.25.** (1) Let  $X$  be a reversible Markov chain.

(2) Let

$$\begin{aligned}\mathbf{X}^1 &= (X_0^1, X_1^1, \dots, X_n^1) \\ &\vdots \\ \mathbf{X}^m &= (X_0^m, X_1^m, \dots, X_n^m)\end{aligned}$$

be  $m$  independent trajectories of length  $n$  from  $X$  starting from a common starting point  $X_0^1 = X_0^2 = \dots = X_0^m = \sigma_0$ .

(3) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(4) Define the random variable  $\mathcal{N}$  to be the number of trajectories  $\mathbf{X}^i$  on which  $\sigma_0$  is an  $\epsilon$ -outlier.

(5) Suppose  $\sigma_0$  is not an  $(\epsilon, \alpha)$ -outlier.

Then

$$\mathbb{P} \left[ \mathcal{N} \geq m \sqrt{\frac{2\epsilon}{\alpha}} + r \right] \leq e^{-r^2 / (2m\sqrt{2\epsilon/\alpha} + r)}.$$

(4)

**Theorem 23.26.** (1) Let  $X$  be a reversible Markov chain.

(2) Let  $n_1, \dots, n_m$  be  $m$  integers independently drawn from a geometric distribution.

(3) Let

$$\begin{aligned}\mathbf{X}^1 &= (X_0^1, X_1^1, \dots, X_{n_1}^1) \\ &\vdots \\ \mathbf{X}^m &= (X_0^m, X_1^m, \dots, X_{n_m}^m)\end{aligned}$$

be  $m$  independent trajectories, each respectively of length  $n_i$ , from  $X$  starting from a common starting point  $X_0^1 = X_0^2 = \dots = X_0^m = \sigma_0$ .

(4) Let  $v : \mathcal{X} \rightarrow \mathbb{R}$  be a value function.

(5) Define the random variable  $\mathcal{N}$  to be the number of trajectories  $\mathbf{X}^i$  on which  $\sigma_0$  is an  $\epsilon$ -outlier.

(6) Suppose  $\sigma_0$  is not an  $(\epsilon, \alpha)$ -outlier.

Then

$$\mathbb{P} \left[ \mathcal{N} \geq m \sqrt{\frac{\epsilon}{\alpha}} + r \right] \leq e^{-r^2 / (m\sqrt{\alpha/(\epsilon)} + r)}.$$

### Vocabulary.

- (1) For a fixed value of  $n$ , the state  $\sigma_0$  is an  $(\epsilon, \alpha)$ -**outlier** in  $\mathcal{X}$  if, among all states in  $\mathcal{X}$ ,  $\rho(0; \epsilon, n \mid \sigma_0)$  is in the largest  $\alpha$  fraction of the values of  $\rho(0; \epsilon, k \mid \sigma_0)$  over all states  $\sigma \in \mathcal{X}$ , weighted according to  $\pi$ . In particular, being an  $(\epsilon, \alpha)$ -outlier measures the likelihood of  $\sigma_0$  failing the local outlier test, ranked against all other states  $\sigma \sim \pi$  of the chain  $X$ .

**Notation.**

- (1)  $n$  – integer number of steps for a Markov chain
- (2)  $X, X_0, X_n$  – Markov chain, starting state, general step of the chain.
- (3)  $\mathcal{X}$  – State space of a Markov chain
- (4)  $v : \mathcal{X} \rightarrow \mathbb{R}$  – value or label function
- (5)  $\pi$  – stationary distribution
- (6)  $x_0$  – a given state from the state space
- (7)  $\sigma_0$  – starting state from the stationary distribution
- (8)  $Y_0, Y_1 \dots$  and  $Z_0, Z_1, \dots$  – two independent trajectories starting from  $Y_0 = Z_0 = \sigma_0$ .
- (9)  $\alpha_0, \alpha_1, \dots, \alpha_n$  – arbitrary real numbers for the definition of outliers
- (10)  $\xi$  – Integer chosen uniformly in  $\{0, \dots, k\}$ .
- (11)  $\epsilon$  – small real number
- (12)  $\rho(j; \ell, n)$  – the probability  $X_j$  is among- $\ell$ -smallest from  $X_0, \dots, X_n$
- (13)  $\rho(j; \ell, n \mid \sigma)$  – the probability  $X_j = \sigma$  is among- $\ell$ -smallest from  $X_0, \dots, X_n$  given the Markov passes through  $\sigma$  at step  $j$
- (14)  $\rho(i; \epsilon, n)$  – the probability that in a  $n$ -step stationary trajectory  $X_0, X_1, \dots, X_k$ ,  $v(X_i)$  is among the smallest  $\epsilon$ -fraction of indices in the list  $v(X_0), v(X_1), \dots, v(X_n)$
- (15)  $\rho(0; \epsilon, k \mid \sigma_0)$  – the probability that on a trajectory  $\sigma_0 = X_0, X_1, \dots, X_n$ ,  $v(\sigma_0)$  is among the smallest  $\epsilon$ -fraction of values in the list  $v(X_0), v(X_1), \dots, v(X_k)$
- (16)  $\mathbf{1}_j$  – the indicator random variable that is 1 whenever  $X_j$  is among- $\ell$ -smallest among  $X_0, \dots, X_n$
- (17) For a fixed value of  $n$ , the state  $\sigma_0$  is an  $(\epsilon, \alpha)$ -**outlier** in  $\mathcal{X}$  if, among all states in  $\mathcal{X}$ ,  $\rho(0; \epsilon, n \mid \sigma_0)$  is in the largest  $\alpha$  fraction of the values of  $\rho(0; \epsilon, k \mid \sigma_0)$  over all states  $\sigma \in \mathcal{X}$ , weighted according to  $\pi$ .
- (18)  $m$  – number of independent trajectories of length  $n$  from  $X$  starting from a common starting point  $X_0^1 = X_0^2 = \dots = X_0^m = \sigma_0$ .
- (19)  $\mathcal{N}$  – the random variable number of trajectories  $\mathbf{X}^i$  on which  $\sigma_0$  is an  $\epsilon$ -outlier.
- (20)  $\rho(j; \epsilon, k \mid \sigma)$  – the probability that  $v(X_j)$  is in the lowest  $\epsilon$  fraction of the values  $v(X_0), \dots, v(X_n)$  conditioned on the event  $X_j = \sigma$ .
- (21)  $\mu$  – mean of a geometric distribution
- (22)  $\mathbf{X} = (X_0^m, X_1^m, \dots, X_k^m)$  – one of  $m$  independent trajectories of length  $n$  from  $X$  starting from a common starting point  $X_0^1 = X_0^2 = \dots = X_0^m = \sigma_0$ .
- (23)  $\rho(0; \epsilon, \mu \mid \sigma)$  – the probability that  $v(X_j)$  is in the lowest  $\epsilon$  fraction of the values  $v(X_0), \dots, v(X_n)$ , conditioned on the event  $X_0 = \sigma$ , where the length  $n$  is chosen from a geometric distribution with mean  $\mu$  supported on  $0, 1, 2, \dots$ ;

### 23.8. Sources

This section is adapted from [CFMP20]. The definition and examples of multiple hypothesis correction is adapted from the Wikipedia article on Multiple comparisons problem

### 23.9. Reading Suggestion:

### 23.10. Outside Readings and Links:

(1)

(2)

(3)

(4)

### 23.11. Algorithms and Scripts

**Input** : Number of balls  $N$  and probability of urn switch,  $p$

**Output**: Alternate Ehrenfest transition probability matrix.

```

1  $N \leftarrow 7, p \leftarrow 1/2, q \leftarrow 1 - p$ 
  // Build  $(N + 1) \times (N + 1)$  transition probability matrix
2  $P_{11} \leftarrow q, P_{12} \leftarrow p$ 
3  $P_{N+1,N} \leftarrow q, P_{N+1,N+1} \leftarrow p$ 
Algorithm. 4 for  $r \leftarrow 2$  to  $N$  do
5    $P_{r,r-1} \leftarrow (r - 1)/N \cdot q$ 
6    $P_{r,r} \leftarrow (N - (r - 1))/N \cdot q + (r - 1)/N \cdot p$ 
7    $P_{r,r+1} \leftarrow (N - (r - 1))/N \cdot p$ 
8 end
```

**Algorithm 21:** Algorithm for defining alternate Ehrenfest transition probability matrix.

**Input** : Number of balls  $N$  and probability of urn switch,  $p$

**Output**: Table of empirical probabilities of  $\epsilon$ -Outlier Test success.

```

1 Build Markov chain object with alternate Ehrenfest matrix
2 Set pathLength, nTrials
3 Initialize matrices to hold Markov chain paths
4 Initialize matrices rhoN rhoN 2ln to hold simulation results
5 foreach element in nTrials do
6   Choose a start state from stationary distribution
7   Create Markov chain path  $X$  and record it
8   foreach  $j \leftarrow 1$  to pathLength +1 do
9     foreach  $l \leftarrow 1$  to pathLength +1 do
10      Increment rhoN entry if  $j$  is among- $l$ -smallest
11    end
12  end
13  Choose a start state from stationary distribution
14  Create independent Markov chain paths  $Y, Z$ 
15  Concatenate  $Y, Z$  and record foreach  $l \leftarrow 1$  to pathLength +1 do
16    Increment rhoN 2ln entry if  $j$  is among- $l$ -smallest
17  end
18 end
19 Divide rhoN and rhoN 2ln by nTrials and report results table
Algorithm 22: Algorithm for simulation of  $\rho$  probabilities in the alternate
Ehrenfest model as an example for understanding.
```

**Input** : Number of balls  $N$  and probability of urn switch,  $p$

**Output**: Table of empirical probabilities of  $\epsilon$ -Outlier Test success.

```

1 Build Markov chain object with alternate Ehrenfest matrix
2 Set pathLength, nTrials
3 Initialize matrices to hold Markov chain paths
4 Initialize matrices rhoN to hold simulation results
5 foreach element in nTrials do
6   Choose a start state from stationary distribution
7   Create Markov chain paths  $Y, Z$  and record them
8   Draw random integer from 1 to pathLength + 1
9   Create random concatenated path
10  foreach  $l \leftarrow 1$  to pathLength + 1 do
11    Increment rhoN entry if  $j$  is among- $l$ -smallest
12  end
13 end
14 foreach  $l \leftarrow 1$  to pathLength + 1 do
15   Increment rhoN 2ln entry if  $j$  is among- $l$ -smallest
16 end
17 Divide rhoN by nTrials and report results probability table
Algorithm 23: Algorithm for simulation of  $\rho$  probabilities in the alternate
Ehrenfest model as an example for understanding.
```

**Input** : Number of balls  $N$  and probability of urn switch,  $p$

**Output**: Table of empirical probabilities of  $\epsilon$ -outlier status for each state.

```

1 Build Markov chain object with alternate Ehrenfest matrix
2 Set pathLength, nTrials
3 Initialize matrices to hold Markov chain paths
4 Initialize matrices rhoCount to hold simulation results
5 foreach state do
6   foreach element in nTrials do
7     Create Markov chain paths from that state and record them
8     Increment rhoCount entry if start state is  $\epsilon$ -outlier
9   end
10 end
11 Divide rhoCount by nTrials and report results probability table
Algorithm 24: Algorithm for simulation of alternate Ehrenfest model as an
example for understanding the definition of  $(\epsilon, \alpha)$ -outlier.
```

### Scripts.

**R:** R script for `simParRhoProb.R`.

```

1 library(markovchain)
2 set.seed(2022)
3
4 N <- 7
```

```

5 p <- 1 / 2
6 q <- 1 - p
7 stateNames <- as.character(0:N)
8 ## Be careful here, because states numbered from 0,
9 ## but R indexes from 1
10 transMatrix <- matrix(0, N + 1, N + 1)
11 transMatrix[1, 1] <- q
12 transMatrix[1, 2] <- p
13 transMatrix[N + 1, N] <- q
14 transMatrix[N + 1, N + 1] <- p
15 for (row in 2:N) {
16   transMatrix[row, row - 1] <- ((row - 1) / N) * q
17   transMatrix[row, row] <- ((N - (row - 1)) / N) * q
18     + ((row - 1) / N) * p
19   transMatrix[row, row + 1] <- ((N - (row - 1)) / N)
20     * p
21 }
22 altEhrenfest <- new("markovchain",
23   transitionMatrix = transMatrix,
24   states = stateNames, name = "AltEhrenfestA"
25 )
26 pathLength <- 10
27 ## pathLength <- 100
28 nTrials <- 15
29
30 recordXPath <- matrix(0, nTrials, pathLength + 1)
31 colnames(recordXPath) <- as.character(0:pathLength)
32 recordYZPaths <- matrix(0, nTrials, 2 * pathLength +
33   1)
34 colnames(recordYZPaths) <- c(
35   paste0("Y", seq(pathLength, 1, -1)),
36   "S0",
37   paste0("Z", seq(1, pathLength))
38 )
39 rhoN <- matrix(0, pathLength + 1, pathLength + 1)
40 rhoN12n <- numeric(pathLength + 1)
41
42 for (i in 1:nTrials) {
43   startState <- as.character(rbinom(1, N, 1 / 2)) #
44     choose start from stable
45   pathX <- markovchainSequence(
46     n = pathLength,
47     altEhrenfest,
48     t0 = startState,

```

```

48     include.t0 = TRUE
49   )
50   recordXPath[i, ] <- as.numeric(pathX)
51   for (j in 1:(pathLength + 1)) {
52     for (l in 1:(pathLength + 1)) {
53       rhoN[j, l] <- rhoN[j, l] + as.numeric((sum((
54         recordXPath[i, ] <= recordXPath[i, j]))) <= 1)
55     }
56   }
57   startState <- as.character(rbinom(1, N, 1 / 2)) #
58   # choose start from stable
59   pathY <- markovchainSequence(
60     n = pathLength,
61     altEhrenfest,
62     t0 = startState,
63     include.t0 = TRUE
64   )
65   pathZ <- markovchainSequence(
66     n = pathLength,
67     altEhrenfest,
68     t0 = startState,
69     include.t0 = FALSE
70   )
71   pathYZ <- c(rev(pathY), pathZ)
72   recordYZPaths[i, ] <- as.numeric(pathYZ)
73   for (l in 1:(pathLength + 1)) {
74     rhoNl2n[l] <- rhoNl2n[l] +
75       as.numeric((sum((recordYZPaths[i, ] <=
76         recordYZPaths[i, pathLength + 1]))) <= 1)
77   }
78 }
79
80 rhoNProb <- rhoN / nTrials
81 rhoNl2nProb <- rhoNl2n / nTrials
82
83 apply(rhoNProb, 2, sum)
84
85 matrix(rep(rhoNl2nProb, 11), 11, 11, byrow = TRUE)
86 matrix(rep(rhoNl2nProb, 11), 11, 11, byrow = TRUE) <=
87   rhoNProb

```

**R:** R script for simBesagClifford.R.

```

1 library(markovchain)
2 set.seed(2022)
3

```



```

4 N <- 7
5 p <- 1 / 2
6 q <- 1 - p
7 stateNames <- as.character(0:N)
8 ## Be careful here, because states numbered from 0,
9 ## but R indexes from 1
10 transMatrix <- matrix(0, N + 1, N + 1)
11 transMatrix[1, 1] <- q
12 transMatrix[1, 2] <- p
13 transMatrix[N + 1, N] <- q
14 transMatrix[N + 1, N + 1] <- p
15 for (row in 2:N) {
16   transMatrix[row, row - 1] <- ((row - 1) / N) * q
17   transMatrix[row, row] <- ((N - (row - 1)) / N) * q
18     + ((row - 1) / N) * p
19   transMatrix[row, row + 1] <- ((N - (row - 1)) / N)
20     * p
21 }
22 altEhrenfest <- new("markovchain",
23   transitionMatrix = transMatrix,
24   states = stateNames, name = "AltEhrenfestA"
25 )
26 pathLength <- 199
27 ## pathLength <- 100
28 nTrials <- 500
29
30 recordRandomYZPath <- matrix(0, nTrials, pathLength +
31   1)
32 colnames(recordRandomYZPath) <- as.character(0:
33   pathLength)
34
35 rhoN <- numeric(pathLength + 1)
36 nEpsOutlier <- 0
37
38 for (i in 1:nTrials) {
39   startState <- as.character(rbinom(1, N, 1 / 2)) #
40     choose start from stable
41   pathY <- markovchainSequence(
42     n = pathLength,
43     altEhrenfest,
44     t0 = startState,
45     include.t0 = TRUE
46   )
47   pathZ <- markovchainSequence(
48     n = pathLength,

```

```

46     altEhrenfest,
47     t0 = startState,
48     include.t0 = TRUE
49 )
50 xi <- sample.int(pathLength + 1, 1) - 1 # 0 to
    pathLength
51 # Caution: R indexes from 1, but Theorem from 0,
    so add 1
52 # Caution: Concatening works if xi <- 0, [1:1] and
    [2:pathLength+1]
53 #         because pathY[1] == pathZ[1], so just
    get pathZ
54 #         But if xi <- pathLength, just want
    pathY, don't concat pathZ[2:1]
55 if (xi < pathLength) {
56     pathRandomYZ <- c(pathY[1:(xi + 1)], pathZ[2:((
    pathLength + 1) - (xi + 1) + 1)])
57 } else { # xi <- pathLength
58     pathRandomYZ <- pathY
59 }
60 recordRandomYZPath[i, ] <- as.numeric(pathRandomYZ)
61 for (l in 1:(pathLength + 1)) {
62     rhoN[l] <- rhoN[l] + as.numeric((sum((
    recordRandomYZPath[i, ] <= recordRandomYZPath[i,
    1]))) <= 1)
63 }
64 # valueStartState <- as.numeric(startState)
65 # if (valueStartState < sort(recordRandomYZPath)[
    outlierThreshold]) {
66 #         nEpsOutlier <- nEpsOutlier + 1
67 # }
68 }
69
70 rhoProb <- rhoN / nTrials
71 probEspOutlier <- nEpsOutlier / nTrials

```

**R:** R script for simEpsAlpha.R.

```

1 library(markovchain)
2 set.seed(2022)
3
4 N <- 7
5 p <- 1 / 2
6 q <- 1 - p
7 stateNames <- as.character(0:N)
8 ## Be careful here, because states numbered from 0,
9 ## but R indexes from 1

```

```

10 transMatrix <- matrix(0, N + 1, N + 1)
11 transMatrix[1, 1] <- q
12 transMatrix[1, 2] <- p
13 transMatrix[N + 1, N] <- q
14 transMatrix[N + 1, N + 1] <- p
15 for (row in 2:N) {
16   transMatrix[row, row - 1] <- ((row - 1) / N) * q
17   transMatrix[row, row] <- ((N - (row - 1)) / N) * q
18   + ((row - 1) / N) * p
19   transMatrix[row, row + 1] <- ((N - (row - 1)) / N)
20   * p
21 }
22 altEhrenfest <- new("markovchain",
23   transitionMatrix = transMatrix,
24   states = stateNames, name = "AltEhrenfest"
25 )
26 pathLength <- 10
27 ## pathLength <- 100
28 nTrials <- 15
29
30 recordPaths <- array(0, dim = c(nTrials, pathLength +
31   1, N + 1))
32 colnames(recordPaths) <- as.character(0:pathLength)
33
34 rhoCount <- numeric(length(stateNames))
35 # rownames(rhoCount) <- as.character(0:pathLength)
36 # colnames(rhoCount) <- as.character(0:pathLength)
37
38 for (startState in 0:N) {
39   for (i in 1:nTrials) {
40     path <- markovchainSequence(
41       n = pathLength,
42       altEhrenfest,
43       t0 = startState,
44       include.t0 = TRUE
45     )
46     valuePath <- as.numeric(path)
47     recordPaths[i, , startState + 1] <- valuePath
48     rhoCount[startState + 1] <-
49       rhoCount[startState + 1] +
50       as.numeric((sum((valuePath <= valuePath[1]))
51         <= 1)
52     )
53   }
54 }

```

```
53 | rhoProb <- rhoCount / nTrials
```

## 23.12. Problems to Work for Understanding

1: Express the slight changes in notation:

- $\rho(j; \epsilon, n)$  is the probability that in an  $n$ -step stationary Markov chain trajectory  $X_0, X_1, \dots, X_n$ ,  $v(X_j)$  is among the smallest  $\epsilon$ -fraction of indices from  $v(X_0), v(X_1), \dots, v(X_n)$ , and
- $\rho(0; \epsilon, k \mid \sigma_0)$  is the probability that in an  $n$ -step stationary Markov chain trajectory  $\sigma_0 = X_0, X_1, \dots, X_n$ ,  $v(\sigma_0)$  is among the smallest  $\epsilon$ -fraction of values in the list  $v(X_0), v(X_1), \dots, v(X_k)$

in terms of the original notations  $\rho(j; \ell, n)$  and  $\rho(j; \ell, n \mid \sigma)$ .

2: Check the Parallel  $2\epsilon$  Test by making some simulations of the alternate Ehrenfest urn model. Use the script to find the proportion of trials for which the starting state, chosen from the stationary distribution, is an 0.01-outlier for the alternative Ehrenfest urn model with  $N = 51$  balls and path length of the chain 199, 399, 599, 999 steps when executing 200, 400, 800 and 1600 trials. Display the results in a  $4 \times 4$  matrix.

3: Check the Besag-Clifford Test by making some simulations of the alternate Ehrenfest urn model. Use the script to find the proportion of trials for which the state 0 is an 0.01-outlier for the alternative Ehrenfest urn model with  $N = 51$  balls and path length of the chain 199, 399, 599, 999 steps when executing 200, 400, 800 and 1600 trials. Display the results in a  $4 \times 4$  matrix.

4: This exercise expands the simulation of the alternate Ehrenfest urn model in `simEpsAlpha.R`. Extend the path length, or number of steps, and the number of trials to sharpen the rough estimates of 0 being an  $(\epsilon, \alpha)$ -outlier.

5: Using a simple internet search, find examples of multiple testing where incorrect conclusions lead to potentially harmful conclusions.



---

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## Solutions

Chapter 1: Markov Chains.

- 1.1: (a) There are 4 states,  $D$  for dropping out, 1 for first-year, 2 for second-year, and  $G$  for graduating.

$$P = \begin{array}{c} \begin{array}{cccc} & D & 1 & 2 & G \\ \begin{array}{c} D \\ 1 \\ 2 \\ G \end{array} & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 3/20 & 1/4 & 3/5 & 0 \\ 1/10 & 0 & 1/5 & 7/10 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \end{array}.$$

- (b) Absorbing states are  $D$  and  $G$ . Transient states are 1, 2.  
(c)

$$P^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 99/400 & 1/16 & 27/100 & 21/50 \\ 3/25 & 0 & 1/25 & 21/25 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Probability of graduating on time is  $21/50$ .

$$P^3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2271/8000 & 1/64 & 183/2000 & 609/1000 \\ 31/250 & 0 & 1/125 & 217/250 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

- (d) Probability of graduating in 3 years is  $609/1000$ .  
(e) Canonical form is

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 3/20 & 0 & 1/4 & 3/5 \\ 1/10 & 7/10 & 0 & 1/5 \end{pmatrix}$$

so

$$N = \begin{pmatrix} 4/3 & 1 \\ 0 & 5/4 \end{pmatrix} \quad B = NA = \begin{pmatrix} 3/10 & 7/10 \\ 1/8 & 7/8 \end{pmatrix}.$$

The chance that a student will graduate eventually is  $7/10$ . The chance the student will drop out eventually is  $3/10$ .

(f) The expected time to graduation is  $4/3 + 1 = 7/3$  years.

Problem created by LT Grant, 2006.

1.2: (a)

$$P = \begin{matrix} & \begin{matrix} A & B & C & D & E & F \end{matrix} \\ \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix} & \begin{pmatrix} 0 & 1/3 & 1/3 & 0 & 1/3 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 1/3 & 1/3 & 0 & 0 & 1/3 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{matrix}.$$

(b) Absorbing states are  $E$  and  $F$ . Transient states are  $A, B, C, D$ .

(c)

$$P' = \begin{matrix} & \begin{matrix} E & F & A & B & C & D \end{matrix} \\ \begin{matrix} E \\ F \\ A \\ B \\ C \\ D \end{matrix} & \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 1/3 & 1/3 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 \\ 0 & 1/3 & 0 & 1/3 & 1/3 & 0 \end{pmatrix} \end{matrix}.$$

$$N = \begin{pmatrix} 2 & 1 & 1 & 1 \\ \frac{3}{2} & 2 & 1 & \frac{3}{2} \\ \frac{3}{2} & 1 & 2 & \frac{3}{2} \\ 1 & 1 & 1 & 2 \end{pmatrix}.$$

(d)  $(N\mathbf{1})_1 = 2 + 1 + 1 + 1 = 5$ .

(e) From  $A$ , probability to  $E$  is  $2/3$ , to  $F$  is  $1/3$ . From  $D$ , probability to  $E$  is  $1/3$ , to  $F$  is  $2/3$ . Seems reasonable by symmetry.

Problem created by LT Grant, 2006.

1.3: (a) Expect absorption probabilities from  $B$  to  $E$  to increase and absorption probability of  $B$  to  $F$  to decrease.

(b) From  $A$ , probability to  $E$  to increase, to  $F$  to decrease. From  $D$ , probability to  $E$  to increase, to  $F$  to decrease.

(c)

$$\begin{pmatrix} 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

- (d) From  $A$ , probability to  $E$  increases to 0.792, to  $F$  decreases to 0.208. From  $D$ , probability to  $E$  increases to approximately 0.458, to  $F$  decreases to approximately 0.542.

Problem created by LT Grant, 2006.

1.4:

$$P_{ij} = \begin{cases} (\frac{i}{N})^2 & j = i - 1, \quad i = 1, 2, \dots, N \\ (2\frac{i}{N})\frac{N-i}{N} & j = i, \quad i = 0, 1, 2, \dots, N \\ 1 - (\frac{i}{N})^2 & j = i + 1, \quad i = 0, 1, 2, \dots, N - 1 \\ 0 & \text{otherwise} \end{cases}$$

There are no absorbing states.

As an example, for  $N = 3$ , the transition probability matrix is

$$\begin{matrix} & 0 & 1 & 2 & 3 \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/9 & 4/9 & 4/9 & 0 \\ 0 & 4/9 & 4/9 & 1/9 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{matrix}$$

with stationary distribution  $\pi = (1/20, 9/20, 9/20, 1/20)$  For  $N = 4$ , the transition probability matrix is

$$\begin{matrix} & 0 & 1 & 2 & 3 & 4 \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1/16 & 6/16 & 9/16 & 0 & 0 \\ 0 & 4/16 & 8/16 & 4/16 & 0 \\ 0 & 0 & 9/26 & 6/16 & 1/16 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \end{matrix}$$

Adapted from Karlin and Taylor, *A First Course in Stochastic Processes*, second edition, page 73, problem 1(b).

1.5:

$$P_{ij} = \begin{cases} (\frac{i}{N})q & j = i - 1, \quad i = 1, 2, \dots, N \\ (\frac{i}{N})p + (\frac{N-i}{N})q & j = i, \quad i = 0, 1, 2, \dots, N \\ (1 - \frac{i}{N})p & j = i + 1, \quad i = 0, 1, 2, \dots, N - 1 \\ 0 & \text{otherwise} \end{cases}$$

An example in the case  $N = 4$

$$\begin{pmatrix} q & p & 0 & 0 & 0 \\ \frac{q}{4} & \frac{3q}{4} + \frac{p}{4} & \frac{3p}{4} & 0 & 0 \\ 0 & \frac{q}{2} & \frac{q}{2} + \frac{p}{2} & \frac{p}{2} & 0 \\ 0 & 0 & \frac{3q}{4} & \frac{q}{4} + \frac{3p}{4} & \frac{p}{4} \\ 0 & 0 & 0 & q & p \end{pmatrix}.$$

The unnormalized stationary distribution is  $[1, 4p/q, 6p^2/q^2, 4p^3/q^3, p^4/q^4]$ , for  $p = 1/2 = q$ , normalized, this is  $[1/16, 1/4, 3/8, 1/4, 1/16]$ , for  $p = 3/4, q = 1/4$ , normalized, this is approximately  $[0.004, 0.047, 0.211, 0.422, 0.316]$ .

There are no absorbing or transient states.



Adapted from Karlin and Taylor, *A First Course in Stochastic Processes*, second edition, page 74, problem 2(a).

1.6:

$$P_{ij} = \begin{cases} (1 - \frac{i}{N})p & j = i - 1, & i = 1, 2, \dots, N \\ (\frac{i}{N})p + (\frac{N-i}{N})q & j = i, & i = 0, 1, 2, \dots, N \\ (\frac{i}{N})q & j = i + 1, & i = 0, 1, 2, \dots, N - 1. \\ 0 & \text{otherwise} \end{cases}$$

There are no absorbing or transient states.

Adapted from Karlin and Taylor, *A First Course in Stochastic Processes*, second edition, page 74, problem 2(b).

1.7: From numerical experiments with the transition probability matrix, slightly more than 50% of the time. This matrix converges fairly slowly to the limiting matrix, so experiments require about  $P^{50}$ .

Adapted from FiveThirtyEight Riddler who in turn got the problem from Steve Simon.

1.8: Keep track of the different “states” of Louie’s umbrellas at home at the end of the work day. He could have 3 at home and 0 at work, 2 at home and 1 at work and so on. In this solution, there are five states: 0, 1, 2 or 3 umbrellas at home plus the state in which Louie has already gotten wet. The rows of the matrix are Louie’s current state, and the columns are his destination. For example, he starts in the third row (2 umbrellas at home and 1 at work). There is no chance he will end the day with zero umbrellas at home since he always has an umbrella available, there is a  $0.3 = 0.5 \cdot 0.6$  chance he will end the day with just 1 at home (from rain in the morning and no rain in the afternoon), a 0.5 chance with 2 at home, a 0.2 chance with 3 at home, and no chance he will get wet on this first day since he always has an umbrella available.

The movement through the random states of a day is described by the transition matrix, which contains the probabilities of umbrellas moving from 1 place to another on any given day. The transition probability matrix is:

$$\begin{pmatrix} 0.3 & 0.2 & 0.0 & 0.0 & 0.5 \\ 0.3 & 0.5 & 0.2 & 0.0 & 0.0 \\ 0.0 & 0.3 & 0.5 & 0.2 & 0.0 \\ 0.0 & 0.0 & 0.3 & 0.5 & 0.2 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{pmatrix}.$$

To get the probabilities for the entire work week, simply multiply this matrix by itself five times, representing the umbrella transitions due to meteorological randomness over the five days, which gives

$$\begin{pmatrix} 0.04791 & 0.07634 & 0.04976 & 0.01776 & 0.80823 \\ 0.11451 & 0.19889 & 0.15274 & 0.06752 & 0.46634 \\ 0.11196 & 0.22911 & 0.22553 & 0.12610 & 0.3073 \\ 0.05994 & 0.15192 & 0.18915 & 0.12425 & 0.47474 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Last, look at the third row (the state in which he began) and the final column: That's the chance he gets wet during the week. Subtract from 1 to find the chance that he didn't get wet and get 69.27 percent.

Adapted from FiveThirtyEight Riddler who in turn got the problem from Josh Vandenharm.) This problem and the solution as a Markov chain appeared in FiveThirtyEight Riddler column of December 14, 2018.

This is a version of Ross, page 181, problem number 22.

1.9: A random walk on the 2-dimensional integer lattice, started off the  $x$ -axis, with the rule that on reaching the  $x$ -axis the chain continues on the  $x$ -axis as a 1-dimensional random walk has an infinite absorbing set, namely the  $x$ -axis. If instead, upon reaching the  $x$ -axis, the chain remains at the hitting point, then the chain has infinitely many absorbing states. This problem is adapted from W. Feller, *An Introduction to Probability Theory and Its Applications*, 3rd Edition, 1957, Jon Wiley and Sons Example XV.4.d, page 386.

Chapter 2: Classes of States and Stationary Distributions.

2.1: (a)

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(b)

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ or } \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

(c)

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(d)

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

State 2 communicates with states 1 and 3, but that is all.

(e)

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

2.2: The 4 states are the number of balls in urn  $A$ , from 0 to 3.

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

In this Markov chain all states communicate, are positive recurrent, are aperiodic, and there are no absorbing or transient states, the Markov chain is irreducible. The stationary distribution is  $\pi = [1/4, 1/4, 1/4, 1/4]$  so in the long run urn  $A$  spends 1/4 of the time empty. This does not depend on the initial distribution of balls.

- 2.3: Label the  $2(n+1)$  states as  $(H, k, n-k)$  or  $(W, k, n-k)$  indicating (redundantly) as starting the trip from Home with  $k$  umbrellas at home, and  $n-k$  umbrellas at Work. Enumerate the states of the Markov chain successively as
- 1::  $(H, 0, n)$  is the state of starting from home with 0 umbrellas at home and  $n$  at work.
  - 2::  $(W, 0, n)$  is the state of starting from work with 0 umbrellas at home and  $n$  at work.
  - : ...
  - $2n-1$ ::  $(H, n-1, 1)$  the state of starting from home with  $n-1$  umbrellas and 1 at work.
  - $2n$ ::  $(W, n-1, 1)$  is the state of starting from work with  $n-1$  umbrellas at home and 1 at work.
  - $2n+1$ ::  $(H, n, 0)$  is the state of starting from home with  $n$  umbrellas at home and 0 at work.
  - $2n+2$ ::  $(W, n, 0)$  is the state of starting from work with  $n$  umbrellas at home and 0 at work.

Then the transition probability matrix is

$$\begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & \dots & 0 & 0 & 0 \\ \dots & & & & & & \\ 0 & 0 & 0 & \dots & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$

It is easiest to examine a small case, say  $n = 3$  and extrapolate from that concrete example. For  $n = 3$ , the probability transition matrix is

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

Then solving  $\pi = \pi \mathbf{P}$  for this small case ( $n = 3$ ) suggests that the solution is  $\pi = (1/(2(2n+1)), 1/(2n+1), \dots, 1/(2n+1), 1/(2(2n+1)))$ . Then it is easy to verify that indeed this is a stationary probability distribution. The professor gets wet when he starts from home with all the umbrellas at work, or starts from work with all the umbrellas at home, (the first and last states) and it is raining. The probability of this, in the long run or asymptotically is

$$\frac{1}{2} \cdot \frac{1}{2(2n+1)} + \frac{1}{2} \cdot \frac{1}{2(2n+1)} = \frac{1}{2(2n+1)}.$$

All states are accessible from each other and therefore the Markov chain is irreducible. It is easy to multiply the transition probability matrix against itself, and see that  $P_{ii}^2 = 1/2$  except for  $i = 2$  and  $i = 2n+1$  where the value is  $3/4$ . Therefore, each state is periodic of period 2.

2.4: The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & 1/2 \\ 0 & 1/2 & 0 & 0 & 1/4 & 1/4 \\ 0 & 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ r/2 & q/2 & p/2 & 0 & 1/2 & 0 \\ r/2 & q/2 & 0 & p/2 & 0 & 1/2 \end{pmatrix} \end{matrix}.$$

The stationary distribution is

$$\left( \frac{r}{2}, \frac{q}{2}, \frac{p(q+2p)}{4}, \frac{p(2r+q)}{4}, \frac{q+2p}{4}, \frac{2r+q}{4} \right).$$

2.5: See the next solution with  $v = 1/3$ .

2.6: Using the assumption that the bathroom is occupied  $1 - v$  of the time, and vacant  $v$  of the time, all day, every day, the transition from state to state each minute is a Markov chain with transition probability

$$\begin{matrix} & O & V \\ \begin{matrix} O \\ V \end{matrix} & \begin{pmatrix} 1-v & v \\ 1-v & v \end{pmatrix} \end{matrix}.$$

It is easy to see that this chain is irreducible, positive recurrent and aperiodic. The stationary distribution is  $(1 - v, v)$ , consistent with the assumption that the bathroom is occupied  $1 - v$  of the time, all day, every day.

The possible transitions at each minute are:

- (1) A Conscientious person is in the bathroom, and it is Occupied and the sign says Occupied. This state is *OCO*. Either the person stays and the state remains Occupied with sign Occupied with probability  $1 - v$ , or the conscientious person leaves and the state is *VV* with probability  $r \cdot v$ .
- (2) A Forgetful person is in the bathroom, and it is Occupied and the sign says Occupied. This state is *OFO*. Either the person stays and the state remains Occupied with sign Occupied with probability  $1 - v$ , or the forgetful person leaves and the state is *VO* with probability  $(1/2) \cdot v = v/2$  or the forgetful person leaves, changing the sign and the state is *VV* with probability  $1/2 \cdot v = v/2$ .
- (3) An Oblivious person is in the bathroom, and it is Occupied and the sign says Occupied. Name this state as *OOO*. Either the person stays and the state remains Occupied with sign Occupied with probability  $1 - v$ , or the oblivious person leaves and the state is *VO* with probability  $v$ .
- (4) A Oblivious person is in the bathroom, and it is Occupied but the sign says Vacant. Name this state as *OOV*. Either the person stays and the state remains Occupied with sign Vacant with probability  $1 - v$ , or the oblivious person leaves and the state is *VV* with probability  $v$ .
- (5) The bathroom is Vacant, but the sign says Occupied. With probability  $1 - v$  some person will approach, nevertheless try the door and find the true state of vacancy and enter, dealing with the sign according to their type. Then the transition is to *OCO* with probability  $r(1 - v)$ , *OFO* with

probability  $q(1-v)$  and  $OOO$  with probability  $p(1-v)$ . With probability  $v$  the state remains  $VO$ .

- (6) The bathroom is Vacant, and the sign says Vacant. With probability  $1-v$  some person will approach, nevertheless try the door and easily find the true state of vacancy and enter, dealing with the sign according to their type. Then the transition is to  $OCO$  with probability  $r(1-v)$ ,  $OFO$  with probability  $q(1-v)$  and  $OOV$  with probability  $p(1-v)$ . With probability  $v$  the state remains  $VV$ .

The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1-v & 0 & 0 & 0 & 0 & v \\ 0 & 1-v & 0 & 0 & v/2 & v/2 \\ 0 & 0 & 1-v & 0 & v & 0 \\ 0 & 0 & 0 & 1-v & v & 0 \\ r(1-v) & q(1-v) & p(1-v) & 0 & v & 0 \\ r(1-v) & q(1-v) & 0 & p(1-v) & 0 & v \end{pmatrix} \end{matrix}.$$

The stationary distribution is:

$$\left( r(1-v), q(1-v), \frac{p(q+2p)(1-v)}{2}, \frac{p(2r+q)(1-v)}{2}, \frac{(q+2p)v}{2}, \frac{(2r+q)v}{2} \right).$$

As  $v \rightarrow 1$ , the stationary distribution tends to  $(0, 0, 0, 0, \frac{(q+2p)}{2}, \frac{(2r+q)}{2})$ . As  $v \rightarrow 0$ , the stationary distribution tends to  $(r, q, \frac{p(q+2p)}{2}, \frac{p(2r+q)}{2}, 0, 0)$ .

- 2.7: Suppose the probability of an oblivious person entering the bathroom is  $w$ . Then proportion of time that the bathroom is occupied by an oblivious person is  $p(1-w)$ . Likewise, and as in the previous problem, the proportion of time the bathroom is occupied by forgetful and conscientious people is  $q(1-v)$  and  $r(1-v)$  respectively. If the probabilities of occupancy by forgetful and conscientious people are both equal to  $1-v$  then the assumption that oblivious people spend twice as much time in the bathroom is  $p(1-w) = 2(q+r)(1-v)$  or  $w = 1 - \frac{2(q+r)}{p}(1-v) = 1 - \frac{2(1-p)}{p}(1-v)$ . Since  $0 < w < 1$ , this puts some restrictions depending on  $p$  and  $v$ .

The transition probability matrix is

$$P = \begin{matrix} & \begin{matrix} OCO & OFO & OOO & OOV & VO & VV \end{matrix} \\ \begin{matrix} OCO \\ OFO \\ OOO \\ OOV \\ VO \\ VV \end{matrix} & \begin{pmatrix} 1-v & 0 & 0 & 0 & 0 & v \\ 0 & 1-v & 0 & 0 & v/2 & v/2 \\ 0 & 0 & 1-w & 0 & w & 0 \\ 0 & 0 & 0 & 1-w & w & 0 \\ r(1-v) & q(1-v) & p(1-v) & 0 & v & 0 \\ r(1-v) & q(1-v) & 0 & p(1-v) & 0 & v \end{pmatrix} \end{matrix}.$$

- 2.8: (1) First consider the statement: If  $i$  and  $j$  communicate, and  $i$  is recurrent, then so is  $j$ .

- (a) If  $i$  and  $j$  communicate, then there is an  $r > 0$  such that  $(P^r)_{ji} > 0$  and an  $s > 0$  such that  $(P^s)_{ij} > 0$ .
- (b) If  $i$  is recurrent, then  $\sum_{n=1}^{\infty} (P^n)_{ii} = \infty$  so also  $\sum_{n=r+s+1}^{\infty} (P^n)_{ii} = \infty$ .
- (c)  $(P^n)_{jj} > (P^r)_{ji}(P^{n-r-s})_{ii}(P^s)_{ij}$ , that is the probability of going from  $j$  to  $j$  is greater than the probability of an excursion from  $j$  to  $i$ , then from  $i$  to  $i$ , and from  $i$  to  $j$ .
- (d) Then

$$\sum_{n=1}^{\infty} (P^n)_{jj} > \sum_{n=r+s+1}^{\infty} (P^r)_{ji}(P^{n-r-s})_{ii}(P^s)_{ij} = (P^r)_{ji} \left( \sum_{n=r+s+1}^{\infty} (P^{n-r-s})_{ii} \right) (P^s)_{ij} = \infty$$

Therefore,  $j$  is recurrent.

- (2) Suppose  $i$  and  $j$  communicate, and  $i$  is transient, but  $j$  is recurrent. Since  $j$  communicates with  $i$  and  $j$  is recurrent, by the previous proof then  $i$  must be recurrent, a contradiction. Therefore,  $j$  must be transient.
- (3) The statement follows from the definition of irreducible and the previous proofs.

2.9: The recursive equation can be interpreted by considering paths for which  $X_0 = i$  and  $X_n = j$  and the first return to state  $j$  occurs at step  $k$ . The probability that the first return is at step  $k$  is  $f_{ij}^k$  and the probability of then going from state  $j$  to state  $j$  in  $n-k$  steps, independent of the past, is  $(P^{n-k})_{jj}$ . Adding over all the disjoint possible first arrivals from  $i$  to  $j$  gives the recursive equation.

2.10: Let  $\epsilon > 0$  be given. Choose  $N_1$  so large that  $|a_n - a| < \epsilon/2$  for  $n > N_1$ . Choose  $N_2 > N_1$  so large that  $\frac{1}{n} \sum_{\nu=1}^{N_1} |a_\nu - a| < \epsilon/2$  for  $n > N_2$ . Then for  $n > N_2$ ,

$$\begin{aligned} \left| \frac{1}{n} \sum_{\nu=1}^n a_\nu - a \right| &\leq \frac{1}{n} \sum_{\nu=1}^{N_1} |a_\nu - a| + \frac{1}{n} \sum_{\nu=N_1+1}^n |a_\nu - a| \\ &\leq \frac{1}{n} \sum_{\nu=1}^{N_1} |a_\nu - a| + \frac{1}{n} \sum_{\nu=N_1+1}^n |a_\nu - a| \\ &< \frac{\epsilon}{2} + \frac{1}{n} \sum_{\nu=N_1+1}^n \frac{\epsilon}{2} \\ &< \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon. \end{aligned}$$

Therefore

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{\nu=1}^n a_\nu = a,$$

2.11: By induction it is enough to prove  $\lim_{j \rightarrow \infty} u_{n_j-1} = \mu$ .

From the hypotheses on  $a_k$  and  $b_k$ , it follows by induction that  $u_n \geq 0$  for all  $n$ . Recall that  $\mu = \liminf_{n \rightarrow \infty} u_n$  with a subsequence such that  $\lim_{j \rightarrow \infty} u_{n_j} = \mu$ .

For purposes of proof by contradiction, suppose that  $\lim_{j \rightarrow \infty} u_{n_j-1} \neq \mu$ . Then there exists a value  $\mu' > \mu$  such that  $u_{n_j-1} > \mu'$  for an infinite number of  $j$ . Let  $\epsilon = \min \{1, a_1(\mu' - \mu)/L\} > 0$  where  $L > \mu + a_1 + 3$ . For the given  $\epsilon$  determine  $N(\epsilon)$  so large that

$$\sum_{k=0}^{N(\epsilon)} a_k > 1 - \epsilon$$

or equivalently

$$\sum_{k=N(\epsilon)+1}^{\infty} a_k < \epsilon$$

Now let  $j$  be chosen so large that  $n_j > N(\epsilon)$  and  $u_{n_j} < \mu + \epsilon$  (possible since  $\lim_{j \rightarrow \infty} u_{n_j} = \mu$ ) and add additionally  $j$  so large that  $u_{n_j-1} > \mu'$  (possible since  $u_{n_j-1} > \mu'$  for an infinite number of  $j$ ) and finally  $u_n > \mu - \epsilon$  for  $n > n_j - N(\epsilon)$  (possible since  $\mu = \liminf_{n \rightarrow \infty} u_n$ ). This set of choices using  $\epsilon$  and  $N(\epsilon)$  establishes a large value of  $j$  with corresponding large  $n_j$ .

Since  $b_n \geq 0$ , the renewal equation implies

$$\begin{aligned} u_{n_j} &\geq \sum_{k=0}^{n_j} a_k u_{n_j-k} \\ &= \sum_{k=0}^{N(\epsilon)} a_k u_{n_j-k} + \sum_{k=N(\epsilon)+1}^{n_j} a_k u_{n_j-k} \\ &\geq \sum_{k=0}^{N(\epsilon)} a_k u_{n_j-k} \\ &= (a_0 u_{n_j} + a_2 u_{n_j-2} + \cdots + a_{N(\epsilon)} u_{n_j-N(\epsilon)}) + a_1 u_{n_j-1} \\ &\geq (a_0 + a_2 + \cdots + a_{N(\epsilon)})(\mu - \epsilon) + a_1 \mu' \\ &> (1 - \frac{\epsilon}{M} - a_1)(\mu - \epsilon) + a_1 \mu' \\ &= \mu - \epsilon \mu - a_1 \mu - \epsilon(1 - \epsilon - a_1) + a_1 \mu' \\ &= \mu + a_1(\mu' - \mu) - \epsilon \mu - \epsilon(1 - \epsilon - a_1) \\ &= \mu + L\epsilon - \epsilon(\mu + 1 - \epsilon - a_1) \\ &= \mu + \epsilon(L - 1 - \epsilon - \mu + a_1) \\ &> \mu + \epsilon(L - 1 - 1 - \mu + a_1). \end{aligned}$$

By the choice of  $L$  the last expression is greater than  $\mu + \epsilon$ , a contradiction, establishing the result.

2.12: It is immediate that  $\pi_1 = \frac{1}{p}\pi_0$ . By induction  $\pi_i = \frac{(1-p)^{i-1}}{p^i}\pi_0$ . The normalization condition is

$$\pi_0 \left( 1 + \frac{1}{p} + \frac{(1-p)}{p^2} + \frac{(1-p)^2}{p^3} + \cdots \right) = 1.$$

Now is apparent why  $p > 1/2$  is necessary for stationarity. The normalization simplifies to  $\pi_0 \left( 1 + \frac{1}{2p-1} \right) = 1$ . Then  $\pi_\nu = \frac{2p-1}{2p} \left( \frac{(1-p)^{\nu-1}}{p^\nu} \right)$  for  $\nu \geq 1$ .

Chapter 3: Waiting Time to Absorption.

3.1: This leads to the single-step transition matrix  $P$  partitioned into one absorbing state for “leave firm” and three transient states: junior lawyer, senior lawyer, partner

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.05 & 0.80 & 0.15 & 0 \\ 0.10 & 0 & 0.70 & 0.20 \\ 0.05 & 0 & 0 & 0.95 \end{pmatrix}.$$

The transient transition matrix is

$$T = \begin{pmatrix} 0.80 & 0.15 & 0 \\ 0 & 0.70 & 0.20 \\ 0 & 0 & 0.95 \end{pmatrix}.$$

The corresponding fundamental matrix is

$$N = (I_3 - T)^{-1} = \begin{pmatrix} 5 & 5/2 & 10 \\ 0 & 10/3 & 40/3 \\ 0 & 0 & 20 \end{pmatrix}.$$

The waiting times to absorption are then

$$(I - T)^{-1}\mathbf{1} = (35/2, 50/3, 20)^T.$$

Now compute the covariances for the first transient state, junior lawyer. Using

$$\text{diag } N_{(1,\cdot)}N + N^T \text{diag } N_{(1,\cdot)} - N_{(1,\cdot)}^T N_{(1,\cdot)} - \text{diag } N_{(1,\cdot)}$$

gives

$$\text{Cov}[Y_{1j}, Y_{1k}] = \begin{pmatrix} 20 & 0 & 0 \\ 0 & 95/12 & 25/3 \\ 0 & 25/3 & 290 \end{pmatrix} = \begin{pmatrix} 20 & 0 & 0 \\ 0 & 7.91667 & 8.33333 \\ 0 & 8.33333 & 290 \end{pmatrix}.$$

Since  $w_i = \sum_{j=a+1}^t Y_{ij}$ , using  $\text{Var}[w_i] = \sum_{j=a+1}^t \sum_{l=a+1}^t \text{Cov}[Y_{1j}, Y_{1l}]$ , the variance is the sum of the entries in the covariance matrix. Hence  $\text{Var}[w_1] = 334.58$  (in units of year<sup>2</sup>). The standard deviation is 18.29 years. As a point of special interest, note that the standard deviation is larger than the mean so that knowing the mean is not enough to understand how long a junior lawyer will be with the firm.

3.2: Theorem 3.3 gives the variances of the waiting times as

$$\text{Var}[\mathbf{w}] = (2N - I)N\mathbf{1} - (N\mathbf{1})_{\text{sq}}.$$

Using the matrix  $N$  from the test example, this is

$$\begin{pmatrix} 551592 \\ 7225 \\ 476496 \\ 7225 \\ 83352 \\ 1445 \\ 15264 \\ 289 \\ 330312 \\ 7225 \\ 247536 \\ 7225 \\ 5400 \\ 289 \end{pmatrix}$$



or approximately

$$\begin{pmatrix} 76.345 \\ 65.951 \\ 57.683 \\ 52.817 \\ 45.718 \\ 34.261 \\ 18.685 \end{pmatrix}$$

The entry for 0 rounds to 52.81661, the same as the variance in the text example.

3.3: For  $1 \leq j \leq 5$ , let  $p_j$  be the probability that the frog eventually reaches pad 10 starting at pad  $j$ . By symmetry  $p_5 = \frac{1}{2}$ . For the frog to reach pad 10 starting from pad 4, the frog goes either to pad 3 with probability  $\frac{2}{5}$  or to pad 5 with probability  $\frac{3}{5}$ , and then continues on a successful sequence from either of these pads. Thus  $p_4 = \frac{2}{5}p_3 + \frac{3}{5}p_5 = \frac{2}{5}p_3 + \frac{3}{10}$ . Similarly, to reach pad 10 starting from pad 3, the frog goes either to pad 2 with probability  $\frac{3}{10}$  or to pad 4 with probability  $\frac{7}{10}$ . Thus  $p_3 = \frac{3}{10}p_2 + \frac{7}{10}p_4$ , and substituting from the previous equation for  $p_4$  gives  $p_3 = \frac{5}{12}p_2 + \frac{7}{24}$ . In the same way,  $p_2 = \frac{1}{5}p_1 + \frac{4}{5}p_3$  and after substituting for  $p_3$  gives  $p_2 = \frac{3}{10}p_1 + \frac{7}{20}$ . Lastly, for the frog to escape starting from pad 1, it is necessary for it to get to pad 2 with probability  $\frac{9}{10}$ , and then escape starting from pad 2. Thus  $p_1 = \frac{9}{10}p_2 = \frac{9}{10}(\frac{3}{10}p_1 + \frac{7}{20})$ , and solving the equation gives  $p_1 = \frac{63}{146}$ .

This problem and solution are from the 2014 AMC 12 B, number 22.

3.4: Use first-step analysis, setting up a system of linear equations in which each variable represents the probability that the goal (in this case, that the frog ends at a vertical side of the square) is achieved from a specific location. In this case there are 9 internal locations, so the system will have 9 variables and 9 equations. Exploiting the symmetry of this problem can reduce the number of variables and equations to 4. Let  $m$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(2, 2)$ ; let  $c$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(1, 3)$ ,  $(3, 3)$ ,  $(3, 1)$ , or  $(1, 1)$ ; let  $v$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(1, 2)$  or  $(3, 2)$ ; and let  $h$  be the probability that the frog ends on a vertical side of the square given that it is currently at  $(2, 1)$  or  $(2, 3)$ . (These letters were chosen to stand for middle, center, vertical, and horizontal, respectively.) Because the probability of a move left, right, down, or up at each step is  $\frac{1}{4}$ , these variables must satisfy the following system:

$$\begin{aligned} m &= \frac{1}{2}v + \frac{1}{2}h \\ c &= \frac{1}{4} + \frac{1}{4}v + \frac{1}{4}h \\ v &= \frac{1}{4} + \frac{1}{4}m + \frac{1}{2}c \\ h &= \frac{1}{2}m + \frac{1}{2}c. \end{aligned}$$

The solution of this system is  $m = \frac{1}{2}$  (which in retrospect is obvious by symmetry),  $c = \frac{1}{2}$  (also obvious by symmetry),  $v = \frac{5}{8}$  (the requested probability), and  $h = \frac{3}{8}$ .

This problem and solution are from the 2020 AMC 12A, number 11.

3.5: The game neither adds nor subtracts the number of balls in use at any turn of the game, so  $a + b + c = n$  is fixed. Then it is sufficient to keep track of the number of balls in urns A and B in any turn. Let  $D_{a,b} = \mathbb{E}[\tau | N_{a,b}]$  be the expected duration of the game when the urn A has  $a$  balls, urn B has  $b$  balls, and urn C has  $c = n - a - b$  balls. Using first-step analysis:

- urn A has  $a + 1$  balls, urn B has  $b - 1$  balls and urn C has  $n - a - b$  balls with probability  $1/6$ ,
- urn A has  $a + 1$  balls, urn B has  $b$  balls and urn C has  $n - a - b - 1$  balls with probability  $1/6$ ,
- urn A has  $a - 1$  balls, urn B has  $b + 1$  balls and urn C has  $n - a - b$  balls with probability  $1/6$ ,
- urn A has  $a$  balls, urn B has  $b + 1$  balls and urn C has  $n - a - b - 1$  balls with probability  $1/6$ ,
- urn A has  $a - 1$  balls, urn B has  $b$  balls and urn C has  $n - a - b + 1$  balls with probability  $1/6$ ,
- urn A has  $a$  balls, urn B has  $b - 1$  balls and urn C has  $n - a - b + 1$  balls with probability  $1/6$ .

Then

$$D_{a,b} = (1/6)[D_{a+1,b-1} + D_{a+1,b} + D_{a-1,b+1} + D_{a,b+1} + D_{a-1,b} + D_{a,b-1}] + 1$$

The boundary conditions are

- (1)  $D_{0,b} = 0$  for  $0 \leq b \leq n$ ,
- (2)  $D_{a,0} = 0$  for  $0 \leq a \leq n$ ,
- (3)  $D_{a,b} = 0$  for  $a + b = n$ .

The solution of this non-homogeneous two-variable difference equation, with these boundary conditions is

$$D_{a,b} = \frac{3}{n}ab(n - a - b).$$

This can be verified by substitution but that leaves open the question of how such a solution is obtained. To motivate the equation by guessing, note that the original problem is symmetric in the urns A, B and C, that is it does not matter which urn is labeled A. In turn, that means the solution must be symmetric in the variables  $a$  and  $b$ . Since the only symmetric polynomials in  $a$  and  $b$  are  $ab$  and  $a + b$ , it makes sense to search for a solution as a combination of these variables. Furthermore, the product  $Kab(n - a - b)$  (where  $K$  is a constant to be determined) satisfies the boundary conditions. Finally, this product is similar to the solution  $a(n - a)$  in the two urn, single variable case. Substituting  $Kab(n - a - b)$  and determining the constant  $K$  reveals the solution.

3.6: The equality is trivial for the base case  $m = 1$ . Assume the equality holds for  $m - 1$ . Check the multiplication for the lower left block, the other three

blocks are easily seen to hold. The multiplication for the lower left block is

$$((I_t + T + T^2 + \cdots + T^{m-2})A)I_a + T^{m-1}A = (I_t + T + T^2 + \cdots + T^{m-1})A.$$

Note  $AI_a = A$ . Using associative and distributive properties for matrix multiplication completes the induction step.

- 3.7: (a) With R, for  $p = 1/2$ ,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.924$ . With R, for  $p = 2/3$ ,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.933$ .  
 (b) With R,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.794$ .  
 (c) With R,  $\text{norm}(T, \text{type}=\text{c}("2")) = 0.866$ .  
 (d) Proof lightly adapted from StackExchange – Substochastic matrix spectral radius For any state  $i$  and integer  $n \geq 0$ , let  $r_i^n = \sum_{\nu} (T^n)_{i\nu}$  denote the  $i$ th row sum of  $T^n$ . For  $n = 1$ , for convenience write  $r_i$  rather than  $r_i^1$ . Since  $T$  is a substochastic transition probability matrix,  $0 \leq r_i^n \leq 1$ . Let  $l^*$  be an index with  $r_{l^*} < 1$ , and note that for  $n \geq 1$

$$r_{l^*}^n = \sum_l T_{l^*l} r_l^{n-1} \leq \sum_l T_{l^*l} = r_{l^*} < 1.$$

By irreducibility, for any  $i$ , there is an  $m$  with  $(T^m)_{il^*} > 0$ . In fact, if  $T$  is an  $N \times N$  matrix, and  $i \neq l^*$  then take  $m < N$ . (Take the shortest path from  $i$  to  $l^*$  with positive transition probability). Since  $(T^m)_{il}$  puts positive weight on the index  $l = l^*$ ,

$$r_i^N = \sum_l T_{il}^m r_l^{N-m} < r_i^m \leq 1.$$

That is, every row sum of  $T^N$  is strictly less than 1. Now it is possible to show  $T^{jN} \rightarrow 0$  as  $j \rightarrow \infty$  and this shows  $T^N$  (and hence  $T$ ) cannot have any eigenvalue with modulus 1.

- (e) Note that if  $\mathbf{x} = (0, 1, 0, 0)^T$ , then  $T\mathbf{x} = (0, 1, 1/2, 0)$  with  $\|T(x)\| = \sqrt{5}/2 \approx 1.118 > 1$ . In fact, With R,  $\text{norm}(T, \text{type}=\text{c}("2")) = 1.162$  but the eigenvalues are 0.833, 0.500, 0 and 0. The previous theorem is not violated because the transient transition probability matrix is not irreducible, it is not possible to reach state 1 + 1 + 1 + 1. Note also the converse of the previous theorem is not true: This matrix has operator norm less than 1, but it is not irreducible.

- 3.8: First note  $NT = TN$  because

$$\begin{aligned} T(I_t - T) &= (I_t - T)T \\ T &= (I_t - T)T(I_t - T)^{-1} \\ (I_t - T)^{-1}T &= T(I_t - T)^{-1} \\ NT &= TN \end{aligned}$$

Start with  $N = (I_t - T)^{-1}$ . Then

$$\begin{aligned}
 I_t &= N(I_t - T) \\
 0 &= N - NT - I_t \\
 T &= N - TN - I_t + T \\
 T &= (I_t - T)N - (I_t - T) \\
 T &= (I_t - T)(N - I_t) \\
 (I_t - T)^{-1}T &= N - I_t
 \end{aligned}$$

3.9: Consider

$$\begin{aligned}
 (I - T)(I + T + T^2 + \cdots + T^m) &= (I + T + T^2 + \cdots + T^m) - \\
 &\quad (T + T^2 + \cdots + T^{m+1}) = I - T^{m+1}
 \end{aligned}$$

Then

$$\|(I - T) \sum_{\nu=0}^m (T^\nu) - I\| = \|T^{m+1}\| \rightarrow 0$$

so

$$\sum_{\nu=0}^{\infty} (T^\nu) = (I - T)^{-1}.$$

3.10: With 1 candle, and the assumption you blow out a random number of candles between one and the number that remain,  $w_1$  must be  $1 = H_1$  and the base case is established. Next assume

$$w_N = H_N = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \cdots + \frac{1}{N} = \sum_{\nu=1}^N \frac{1}{\nu}.$$

The first-step equation is

$$\begin{aligned}
 w_{N+1} &= 1 + \frac{1}{N+1}w_1 + \frac{1}{N+1}w_2 + \cdots + \frac{1}{N+1}w_N \\
 &= 1 + \frac{1}{N+1} \sum_{\nu=1}^N w_\nu \\
 &= 1 + \frac{1}{N+1} \sum_{\nu=1}^{N+1} \sum_{j=1}^{\nu} \frac{1}{j} \\
 &= 1 + \frac{1}{N+1} \sum_{j=1}^N \frac{N-(j-1)}{j} \\
 &= 1 + \frac{1}{N+1} \sum_{j=1}^N \left( \frac{N+1}{j} - 1 \right) \\
 &= 1 + \sum_{j=1}^N \frac{1}{j} - \frac{1}{N+1}(N) \\
 &= \sum_{j=1}^N \frac{1}{j} + \frac{1}{N+1} \\
 &= w_{N+1}
 \end{aligned}$$

Chapter 4: Standard Examples.

4.1: (a) For the first Ehrenfest model

$$P_{ij} = \begin{cases} i/k & \text{if } j = i - 1, \\ (k-i)/k & \text{if } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$

(b) For the second Ehrenfest model

$$P_{ij} = \begin{cases} \frac{i}{k}q & \text{if } j = i - 1, \\ \frac{i}{k}p + \frac{k-i}{k}q & \text{if } j = i, \\ \frac{k-i}{k}p & \text{if } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$

(c) For the third Ehrenfest model

$$P_{ij} = \begin{cases} \frac{k-i}{k}p & \text{if } j = i - 1, \\ \frac{i}{k}p + \frac{k-i}{k}q & \text{if } j = i, \\ \frac{i}{k}q & \text{if } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$

(d) For the fourth Ehrenfest model

$$P_{ij} = \begin{cases} \frac{i(k-i)}{k^2} & \text{if } j = i - 1, \\ \frac{i^2}{k^2} + \frac{(k-i)^2}{k^2} & \text{if } j = i, \\ \frac{i(k-i)}{k^2} & \text{if } j = i + 1, \\ 0 & \text{otherwise.} \end{cases}$$

4.2: Entry  $i$  must satisfy

$$\binom{k}{i-1} \left(\frac{1}{2}\right)^k \cdot \frac{k-i+1}{k} + \binom{k}{i+1} \left(\frac{1}{2}\right)^k \cdot \frac{i+1}{k} = \binom{k}{i} \left(\frac{1}{2}\right)^k$$

or more simply

$$\binom{k}{i-1} \cdot \frac{k-i+1}{k} + \binom{k}{i+1} \cdot \frac{i+1}{k} = \binom{k}{i}.$$

This reduces to

$$\binom{k-1}{i-1} + \binom{k-1}{i+1} = \binom{k}{i}.$$

which is the basic binomial (Pascal triangle) identity.

4.3: Using the probability transition matrix from `ehrfest3.R` and using the `markovchain` package in R:

```
R> absorptionProbabilities(ehrenfest3)
      0      7
1 0.984375 0.015625
2 0.890625 0.109375
3 0.656250 0.343750
4 0.343750 0.656250
5 0.109375 0.890625
6 0.015625 0.984375
R> meanAbsorptionTime(ehrenfest3)
      1      2      3      4      5      6
3.033333 7.233333 10.733333 10.733333 7.233333 3.033333
```

Using the probability transition matrix from `ehrfest4.R` and using the `markovchain` package in R:

```
R> absorptionProbabilities(ehrenfest4)
      0      7
1 0.8571429 0.1428571
2 0.7142857 0.2857143
3 0.5714286 0.4285714
4 0.4285714 0.5714286
5 0.2857143 0.7142857
6 0.1428571 0.8571429
R> meanAbsorptionTime(ehrenfest4)
      1      2      3      4      5      6
17.15000 26.13333 30.21667 30.21667 26.13333 17.15000
```

$$P = \begin{pmatrix} 1-p & p & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$
$$(\boldsymbol{\pi}_{1,0}, \boldsymbol{\pi}_{0,1}, \boldsymbol{\pi}_{0,2}) = \left( \frac{1}{1+2p}, \frac{p}{1+2p}, \frac{p}{1+2p} \right).$$

4.6: The state space is the set of nonnegative integers. At time period  $t$ , suppose there are  $i$  infected individuals not in quarantine. Suppose that  $j$  ( $0 \leq j \leq i$ ) of these contagious individuals infect another  $j$  individuals and that  $i - j$  are discovered and moved to quarantine. At the next time period there are a net number  $i + j - (i - j) = 2j$  infectives in the population with probability  $\binom{i}{j} p^j (1 - p)^{i-j}$ . This is a discrete time Markov chain on an infinite state space with transition probability  $p_{i\ell} = \binom{i}{\ell/2} p^{\ell/2} (1 - p)^{i-(\ell/2)}$  for  $i \geq 0$  and  $0 \leq \ell \leq 2i$  and  $\ell$  even.

The probability that by period 1 the one carrier has not been discovered is  $p$ , by period 2 there are 2 carriers and the probability that each is not yet discovered is  $p^2$ , by period three there are 4 carriers with no discoveries with probability  $p^4$ , and by period  $n$  there are  $2^{n-1}$  carriers with no discoveries  $p^{2^{n-1}}$ .

Chapter 5: The Game of Monopoly as a Markov Chain.

```

1 library("markovchain")
2
3 rotvec <- function(vec) vec[ c(length(vec), 1:(length
4 (vec)-1)) ]
5
6 nStates <- 8
7 monopolyStates <- as.character( c(1:nStates) )
8
9 diceRoll <- matrix(0, nStates, nStates)
10
11 p1 <- c(0, 1/2, 1/2, 0, 0, 0, 0, 0)
12
13 for (i in 1:nStates) {
14   diceRoll[i, ] <- p1
15   p1 <- rotvec(p1)
16 }
17
18 Jail <- diag(nStates)
19 Jail[4, 4] <- 0
20 Jail[4, 2] <- 1
21
22 #go from Police
23   to Jail

```

```

19 |
20 | Ch <- diag(nStates)
21 | Ch[6, 7] <- 1/16                      #Nearest
   |     Railroad
22 | Ch[6, 8] <- 1/16                      #Advance to
   |     Go
23 | Ch[6, 1] <- 1/16                      #Reading
   |     Railroad
24 | Ch[6, 2] <- 1/16                      #Go to Jail
25 | Ch[6, 3] <- 1/16                      #Go back 3
26 | Ch[6, 6] <- 11/16                    #All other
   |     cards
27 |
28 | monopolMat <- diceRoll %*% Jail %*% Ch
29 |
30 | mcMonopoly8 <- new("markovchain", states =
   |     monopolyStates, byrow = TRUE,
31 |                   transitionMatrix = monopolMat, name =
   |     "Monopoly")
32 | ss <- steadyStates(mcMonopoly8)
33 | cat(ss, "\n")

```

```

      1 0.07731016
      2 0.383806
      3 0.2342177
The stationary distribution is 4 0.0
      5 0.1171089
      6 0.04025618
      7 0.08234218
      8 0.06495883

```

Chapter 6: The Game of Risk as a Markov Chain.

6.1: For  $Y^{(1)} = y^{(1)}$ ,  $Y^{(2)} = y^{(2)}$  with  $y^{(1)} > y^{(2)}$ , the individual die values *in some order* must be  $y^{(1)}$ ,  $y^{(2)}$  and  $y^{(3)} \leq y^{(2)}$ . There are 6 orders for each of the  $y^{(2)}$  possibilities for  $y^{(3)}$ , each with probability  $\frac{1}{6^3}$ . However, if  $y^{(3)} = y^{(2)}$ , then the 6 orders are counted twice, so half of them, specifically 3, must be subtracted from the total.

6.2: Count the ways it is possible to have  $Y^{(1)} = y^{(1)}$ . There is 1 way to have  $y^{(1)} = Y^{(1)} = Y^{(2)} = Y^{(3)}$ . There are  $y^{(1)} - 1$  ways to have  $y^{(1)} = Y^{(1)} = Y^{(2)} > Y^{(3)}$  in 3 possible permutations each. There are  $(y^{(1)} - 1)(y^{(1)} - 2)$  ways to have  $y^{(1)} = Y^{(1)} > Y^{(2)} > Y^{(3)}$  in 6 possible permutations each. Each way has probability  $\frac{1}{216}$  so after expanding and simplifying

$$\mathbb{P}[Y^{(1)} = y^{(1)}] = \frac{1 - 3y^{(1)} + 3(y^{(1)})^2}{216}$$

for  $y^{(1)} = 1, 2, 3, 4, 5, 6$ .



6.3: Use the order statistic probability

$$\mathbb{P}[Y^{(1)} = y^{(1)}] = (1 - 3y^{(1)} + 3(y^{(1)})^2)/216.$$

The possibilities for the defender to lose one army are the following:

- (a) The largest die of the 3 rolled by the attacker is a 2, and the value rolled by the defender is 1; occurring with probability  $\frac{7}{216} \cdot \frac{1}{6} = \frac{7}{1296}$ .
- (b) The largest die of the 3 rolled by the attacker is a 3, and the value rolled by the defender is 1 or 2; occurring with probability  $\frac{19}{216} \cdot \frac{2}{6} = \frac{38}{1296}$ .
- (c) The largest die of the 3 rolled by the attacker is a 4, and the value rolled by the defender is 1 or 2 or 3; occurring with probability  $\frac{37}{216} \cdot \frac{3}{6} = \frac{111}{1296}$ .
- (d) The largest die of the 3 rolled by the attacker is a 5, and the value rolled by the defender is 1, 2, 3, or 4; occurring with probability  $\frac{61}{216} \cdot \frac{4}{6} = \frac{244}{1296}$ .
- (e) The largest die of the 3 rolled by the attacker is a 6, and the value rolled by the defender is 1, 2, 3, 4, or 5; occurring with probability  $\frac{91}{216} \cdot \frac{5}{6} = \frac{455}{1296}$ .
- (f) The total probability is  $(7 + 38 + 111 + 244 + 455)/1296 = 855/1296$  (which reduces to  $95/144$ ).

	20	19	18	17	16
	4.441	4.277	4.111	3.943	3.773
	15	14	13	12	11
6.4:	3.601	3.427	3.249	3.068	2.883
	10	9	8	7	6
	2.692	2.498	2.293	2.085	1.854
	5	4	3	2	1
	1.631	1.335	1.110	0.590	0.417

Chapter 7: Games.

7.1: The transition probability matrix for *Tenzi* (rounded to three decimal places) is written in Maxima as

```
pi[i,j] := if (j >= i) then binomial(11-i, j-i) * ((1/6)^(j-i)) *
((5/6)^(11-j)) else 0;
P : genmatrix(pi, 11, 11);
fpprintprec : 3;
float(P);
```

Transfer this matrix of values to R and evaluate with the following script:

```
x <- c(0.1615055828898457, 0.3230111657796915, 0.2907100492017223,
0.1550453595742519, 0.05426587585098816, 0.01302381020423716,
0.002170635034039527, 2.48072575318803*10^-4,
1.860544314891023*10^-5, 8.2690858439601*10^-7,
1.65381716879202*10^-8, 0.0, 0.1938066994678149,
0.3488520590420667, 0.2790816472336534, 0.1302381020423716,
0.03907143061271148, 0.007814286122542296,
0.001041904816338973, 8.930612711476907*10^-5,
4.465306355738455*10^-6, 9.922903012752121*10^-8, 0.0, 0.0,
0.2325680393613778, 0.3721088629782046, 0.2604762040847432,
0.1041904816338973, 0.02604762040847432, 0.004167619265355891,
4.167619265355891*10^-4, 2.381496723060509*10^-5,
```

```

5.953741807651273*10^-7,0.0, 0.0, 0.0, 0.2790816472336534,
0.3907143061271148, 0.2344285836762689, 0.07814286122542295,
0.01562857224508459, 0.001875428669410151,
1.250285779606767*10^-4, 3.572245084590763*10^-6,0.0, 0.0,
0.0, 0.0, 0.3348979766803841, 0.4018775720164609,
0.2009387860082305, 0.05358367626886145, 0.008037551440329218,
6.430041152263375*10^-4, 2.143347050754458*10^-5,0.0, 0.0,
0.0, 0.0, 0.0, 0.4018775720164609, 0.4018775720164609,
0.1607510288065844, 0.03215020576131687, 0.003215020576131687,
1.286008230452675*10^-4,0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.4822530864197531, 0.3858024691358025, 0.1157407407407407,
0.0154320987654321, 7.716049382716049*10^-4,0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.5787037037037037, 0.3472222222222222,
0.06944444444444445, 0.004629629629629629,0.0, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.6944444444444444, 0.2777777777777778,
0.0277777777777778,0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
0.0, 0.8333333333333334, 0.1666666666666667,0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0)
P <- t( matrix(x, 11, 11) )

PPow <- P
tenzicdf <- c(PPow[1,11])
for (i in 2:50) {
  PPow <- PPow %*% P;
  tenzicdf <- c(tenzicdf, PPow[1,11])
}

library(ggplot2)
ggplot(data = as.data.frame(tenzicdf), aes(x=1:50, y=tenzicdf))
+ geom_point()
+ geom_line()

tenzipdf <- tenzipdf[2:50] - tenzipdf[1:49]
tenzipdf <- c(tenzicdf[1], tenzipdf)
ggplot(data = as.data.frame(tenzipdf), aes(x=1:50, y=tenzipdf))
+ geom_point()
+ geom_line()

sum(tenzipdf)
tenzimean <- (1:50) %*% tenzipdf

Q <- P[1:10, 1:10]
I10 <- ident(10)
N <- solve( I10 - Q, I10)
N %*% rep(1,10)

Varw <- ((2 * N - I10) %*% N) %*% rep(1, 10) - ( N %*% rep(1, 10) )^2

```

```
sdw <- sqrt(Varw)
```

7.2: (1) Denote as  $P(n, j)$  the probability that the minimum value from  $n$  random samples of  $p(j)$  is less than or equal to  $j$ . Then  $P(n, j)$  is the complement of the probability that all  $n$  random samples (which are independent of each other) are greater than  $j$ , so  $P(n, j) = 1 - (1 - P(j))^n$ . The p.d.f. giving the probability that a game with  $n$  players is won in exactly  $j$  rolls is  $p(n, j) = P(n, j) - P(n, j - 1)$ .

(2) The expected number of turns in a game of Tenzi with 2 players is 11.897, with 3 players is 10.408, and with 4 players is 9.542.

7.3: A possible path is to roll a 1, to 38; roll a 6, to 44; roll a 6, to 50; roll a 1, to 67; roll a 6, to 73; roll a 6, to 79 and finally, roll a 1 to ascend from 80 to 100. Examination of the first 6 powers of the transition probability matrix show that the probability of 6 step paths from 38 is 0.007265947 but 0 for fewer than 6 steps.

Another possible path is roll a 4, to 14; roll a 6, to 20; roll a 6, to 26; roll a 2, to 84; roll a 6, to 90; roll a 5, to 75 and finally, roll a 5 to ascend from 80 to 100. Examination of the first 6 powers of the transition probability matrix show that the probability of 6 step paths from 14 is 0.001800412 but 0 for fewer than 6 steps.

7.4: (a) The expected length of a game with no chutes or ladders is 31.1 with a standard deviation of 5.98.

(b) The expected length of the game drops from about 39.2 to about 29.8 with a standard deviation of about 18.8.

(c) The game lengthens to about 45.8 moves with a standard deviation of about 33.4.

(d) Lengthens the expected playing time by more than two moves to about 41.9, since it increases the chances of missing the important ladder from state 80 to 100.

(e) Shortens the game by over a move to about 38.0, since it gives a second chance at the long ladder from 28 to 84.

7.5: The win probability if only square 2 is blue is 0.5288 The win probability if squares 2, 3 and 5 are blue is 0.7761. The remaining questions make a good project for student investigation.

7.6: First build some general Julia code to create the transition probability matrices for any  $n$ . This general code does not need the specialized Markov chain packages, but does use the **Graphs** package to check for dominance cycles.

```
1 function markov(size::Integer)
2     idx2states = vec(join.(Iterators.product([ 'h', 't' ] for _ in 1:size)...))
3     states2idx = Dict{idx2states => eachindex(idx2states)}
4     P = zeros(2^size, 2^size)
5     for state in idx2states
6         for next in ("h", "t")
7             nextstate = chop(state, head=1, tail=0) *
            next
```

```

8         P[states2idx[state], states2idx[nextstate]
9         ]] = 0.5
10         end
11     end
12     return P, idx2states, states2idx
end

```

- (1) The `idx2states` vector keeps track of all H and T sequences that have length  $n$  (i.e. it is a mapping from state number to state signature).
- (2) `states2idx` is an inverse mapping from state signature to state number.
- (3) `P` is the transition probability matrix of the chain. Note that from the sequence AB ... (where all elements are H or T) we go to sequence B ...H or B dots T with equal probability.

Next some general code to make Alice and Bob's chosen sequences the absorbing states for game. Instead of rearranging to canonical form and finding the absorption probabilities, make  $2^{32}$  steps of the process (fortunately in Julia it is fast by 5 matrix squarings). Observe that initially all states are equally probably, so the `terminal` matrix keeps information about long term probabilities of staying in all possible states.

```

1 function game(P, states2idx, alice, bob)
2     P_game = copy(P)
3     alice_idx, bob_idx = states2idx[alice],
4     states2idx[bob]
5     P_game[alice_idx, :] .= 0.0
6     P_game[alice_idx, alice_idx] = 1.0
7     P_game[bob_idx, :] .= 0.0
8     P_game[bob_idx, bob_idx] = 1.0
9     n = length(states2idx)
10    terminal = fill(1 / n, 1, n) * P_game^(2^32)
11    return terminal[states2idx[alice]], terminal[
12    states2idx[bob]]
end

```

Finally some code to analyze the game.

```

1 using Graphs
2
3 function analyze_game(size::Integer, details::Bool=
4     true)
5     P, idx2states, states2idx = markov(size)
6     g = SimpleDiGraph(length(states2idx))
7     details && println("\nWinners:")
8     for alice in idx2states, bob in idx2states
9         alice > bob || continue
10     end
11 end

```

```

9      alice_win, bob_win = game(P, states2idx,
alice, bob)
10     if alice_win > 0.51
11         winner = "alice"
12         add_edge!(g, states2idx[alice],
states2idx[bob])
13     elseif bob_win > 0.51
14         winner = "bob"
15         add_edge!(g, states2idx[bob], states2idx[
alice])
16     else
17         winner = "tie (or close)"
18     end
19     details && println(alice, " vs ", bob, ": ",
winner)
20 end
21 cycles = simplecycles(g)
22 if !isempty(cycles)
23     min_len = minimum(length, cycles)
24     filter!(x -> length(x) == min_len, cycles)
25 end
26 println("\nCycles:")
27 for cycle in cycles
28     println(idx2states[cycle])
29 end
30 end

```

```

(1)
1     game2 = markov(2)
2     P = game2[1]
3     game(P, states2idx, "th", "hh")
4     game(P, states2idx, "th", "hh")
5

```

Alice wins with probability 0.75, Bob wins with probability 0.25.

```

(2)
1     game3 = markov(3)
2     P = game3[1]
3     states2idx = game3[3]
4     game(P, states2idx, "tth", "hhh")
5

```

Alice wins with probability 0.7, Bob wins with probability 0.3.

(3) `analyze_game(3)` The shortest cycle has length 4 and it is unique.

Winners:

```

thh vs hhh: alice
thh vs hth: tie (or close)
thh vs hht: alice
thh vs htt: tie (or close)
hth vs hhh: alice
hth vs hht: bob
tth vs hhh: alice
tth vs thh: alice
tth vs hth: alice
tth vs hht: tie (or close)
tth vs tth: alice
tth vs htt: bob
hht vs hhh: tie (or close)
tth vs hhh: alice
tth vs thh: tie (or close)
tth vs hth: tie (or close)
tth vs hht: bob
tth vs htt: tie (or close)
htt vs hhh: alice
htt vs hth: tie (or close)
htt vs hht: bob
htt vs htt: tie (or close)
ttt vs hhh: tie (or close)
ttt vs thh: bob
ttt vs hth: bob
ttt vs tth: tie (or close)
ttt vs hht: bob
ttt vs tth: bob
ttt vs htt: bob

```

Cycles:

```

["thh", "hht", "htt", "tth"]

```

- (4) `analyze_game(4, false)` shows 14 cycles of length 3, shorter than the unique cycle for  $n = 3$ !

This problem and the code for the solution is from <https://bkamins.github.io/julialang/2024/06/14/probability>

- 7.7: (a) For this question, the rounds don't matter at all. The game will end once there is at least 1 correct ball in each cup, and the pruning phase at the end of each round only removes incorrect balls so effectively neglects pruning.

This is a classical coupon collector problem. Define  $Y_i$ , for  $i$  from 0 to  $N - 1$ , to be the number of additional tosses that need to be obtained after  $i$  distinct cups have been filled with corresponding numbered balls. Define  $Y$  as the total number of tosses required to fill the cups with correspondingly numbered balls so

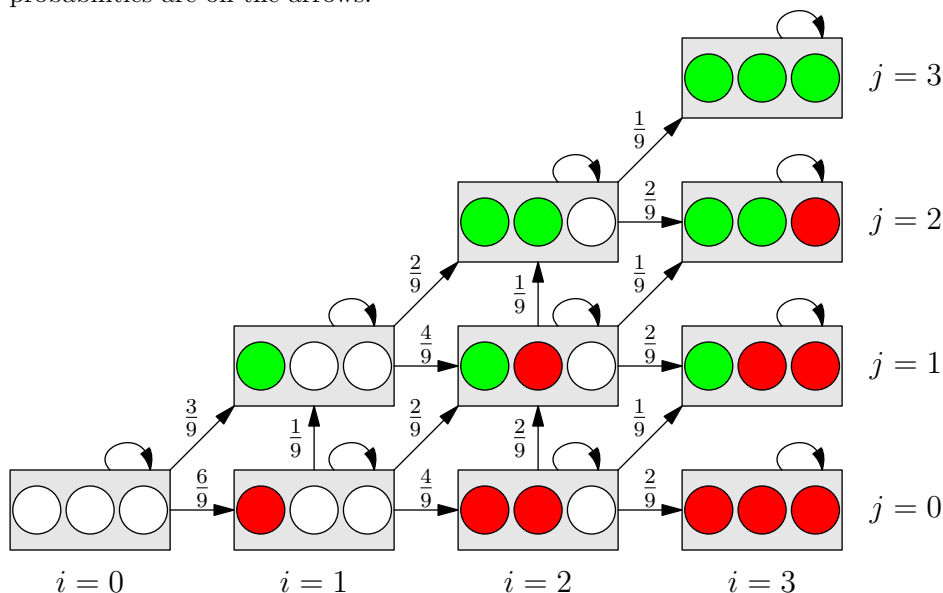
$$Y = Y_0 + Y_1 + Y_2 + \cdots + Y_{N-1}.$$

When  $i$  distinct cups have been filled with corresponding numbered balls, the probability that a ball with a number of an unfilled cup is drawn is  $\frac{N-i}{N}$ . Each time a ball is thrown, there is a  $1/N$  chance it will land in the correct cup. It follows that the probability of success in filling a new cup with the correctly numbered ball is  $\frac{N-i}{N} \cdot \frac{1}{N}$ . Thus,  $Y_i$  is a geometric random variable with success parameter  $\frac{N-i}{N^2}$ . Then  $\mathbb{E}[Y_i] = \frac{N^2}{N-i}$ . Therefore

$$\begin{aligned}\mathbb{E}[Y] &= \mathbb{E}[Y_0] + \mathbb{E}[Y_1] + \mathbb{E}[Y_2] + \cdots + Y_{N-1} \\ &= N + \frac{N^2}{N-1} + \frac{N^2}{N-2} + \cdots + \frac{N^2}{1} \\ &= N^2 \sum_{\nu=1}^N \frac{1}{\nu} \approx N^2(\log N + \gamma)\end{aligned}$$

where  $\gamma \approx 0.577$  is the Euler-Mascheroni constant.

- (b) In general the number of rounds to end the game is complicated, so to illustrate the approach solve it for the case  $N = 3$ . Begin by breaking each round into a number of stages. Each stage tracks the progress of cups as they are filled. In the diagram below, each cup is either empty (no ball), is red (incorrect ball), or is green (correct ball). The transition probabilities are on the arrows.



The integer  $i$  indicates the number of balls thrown. The integer  $j$  indicates the number of cups filled holding a correspondingly numbered ball. A colored cup may contain more than 1 ball. The cup position left to right is not associated with the cup or ball numbers, the position merely indicates the number of correctly or incorrectly filled cups. For example, if 2 balls have been thrown into 2 cups, 1 correctly numbered, 1 incorrectly numbered, the center diagram at  $i = 2, j = 1$  illustrates this case. Then

on the next ball thrown, that ball can incorrectly go into the empty cup with probability  $\frac{N-1}{N} \cdot \frac{1}{N} = \frac{2}{9}$ . The ball can go into the correct cup with probability  $\frac{1}{N}$ . In this diagram, self-loops have whatever probability is required so that the outgoing arrows sum to 1. This is a Markov chain. Start on the initial state at the lower left (all cups empty,  $i = 0, j = 0$ ), and advance to an absorbing state at the right, all cups full with  $i = 3$ . Label the states by columns from top to bottom from right to left. This unusual ordering puts the transition matrix in canonical form. The transition matrix for  $N = 3$  is:

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{9} & \frac{2}{9} & 0 & 0 & \frac{6}{9} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{9} & \frac{2}{9} & 0 & \frac{1}{9} & \frac{5}{9} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{9} & \frac{2}{9} & 0 & \frac{2}{9} & \frac{4}{9} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{9} & \frac{4}{9} & 0 & \frac{3}{9} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{9} & \frac{4}{9} & \frac{1}{9} & \frac{2}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{9} & \frac{6}{9} & 0 \end{pmatrix}.$$

The matrix  $N = (I - T)^{-1}$  is:

$$N = \begin{pmatrix} \frac{3}{1} & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{3} & \frac{9}{4} & 0 & 0 & 0 & 0 \\ \frac{3}{3} & \frac{9}{4} & \frac{9}{5} & 0 & 0 & 0 \\ \frac{3}{3} & \frac{10}{3} & \frac{3}{5} & 0 & 0 & 0 \\ \frac{37}{35} & \frac{48}{35} & \frac{36}{35} & \frac{3}{5} & \frac{9}{7} & 0 \\ \frac{48}{35} & \frac{89}{70} & \frac{34}{35} & \frac{14}{9} & \frac{6}{7} & 1 \end{pmatrix}$$

and

$$B = NA = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 & 0 \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{2} & 0 \\ \frac{1}{30} & \frac{1}{6} & \frac{2}{5} & \frac{2}{5} \\ \frac{1}{6} & \frac{1}{2} & \frac{1}{3} & 0 \\ \frac{1}{15} & \frac{2}{7} & \frac{44}{105} & \frac{8}{35} \\ \frac{1}{10} & \frac{1}{14} & \frac{41}{105} & \frac{16}{105} \end{pmatrix}.$$

The  $ij$  entry in  $B$  gives the probability of going from state  $i+4$  to absorbing state  $j = 1, 2, 3, 4$ .

Being in absorbing state  $j$  means the throwing phase of the round ends and the pruning phase of the round begins. Absorbing state 1 requires no pruning, the round is finished. Absorbing state 2 transitions to state 5, state 3 transitions to state 8 and state 4 transitions to state 10 and the throwing part of the next round resumes.

Now let  $E_5, E_8, E_{10}$  be the expected number of rounds played to end the game starting from states 5, 8, 10 respectively. The main interest is  $E_{10}$  which answers the question. Using first-step analysis, these expected



	<i>AB</i>	<i>S</i>	<i>D</i>	<i>T</i>	<i>HR</i>	<i>BB</i>	<i>AVE</i>	<i>SA</i>	<i>OB</i>	<i>OPS</i>
Ruth	8399	1517	506	136	714	2062	0.342	0.690	0.474	1.164
Williams	7706	1537	525	71	521	2021	0.344	0.634	0.481	1.114

**Table 0.3.** Statistics for Babe Ruth and Ted Williams.

values satisfy the equations

$$\begin{aligned}
 E_5 &= 1 + \frac{2}{3}E_5 \\
 E_8 + 1 + \frac{1}{2}E_5 + \frac{1}{3}E_8 \\
 E_{10} &= 1 + \frac{5}{14}E_5 + \frac{41}{105}E_8 + \frac{16}{105}E_{10}.
 \end{aligned}$$

Solving numerically,  $E_5 = 3$ ,  $E_8 = 3.75$ ,  $E_{10} = 4.171$ .

This problem and the solution as a Markov chain appeared in FiveThirtyEight Riddler column of November 16, 2018. The solution and solution figures are adapted from Five Thirty Eight Riddler.

Chapter 8: A Markov Chain Model of Baseball.

8.1: In 2019, Strasburg was a pitcher for the Washington Nationals in the National League, as he had been since 2010. As a pitcher, his hitting skills and run production are not emphasized, it is his pitching that makes him a valuable player. Furthermore, as a pitcher, he appears in fewer games with even fewer plate appearances. That means he has a smaller base of hitting statistics for creating the matrix  $P$  so  $P$  may not fully reflect his hitting skills.

8.2: Using the script with Trout's statistics, the expected time to absorption starting from the first state of no-outs is 5.22 at-bats per half-inning.

8.3: In the  $25 \times 25$  matrix  $P_K$ , all entries are 0 except for the following:

- For each  $i$ ,  $i = 1, \dots, 25$  and  $j = 1, 2, 3$  with  $j = i \bmod 3$ ,  $(P_K)_{ij} = q$ ,
- For each  $i$ ,  $i = 1, \dots, 25$  with  $i \neq 0 \bmod 3$ , and  $j = i + 1$   $(P_K)_{ij} = 1 - q$
- For each  $i$ ,  $i = 1, \dots, 25$  with  $i = 0 \bmod 3$  and  $j = 25$   $(P_K)_{ij} = 1 - q$ .

In the special case  $q = 0.1$ , the Markov runs statistic for a half-inning is 0.333 and the markov RPG is 3.

8.4: Using the 2024 data for Aaron Judge, 2024 American League MVP, his markovRPG is 11.8.

8.5: The lifetime career statistics for Babe Ruth (1914–1935) and Ted Williams (1939–1942, 1946–1960) are in Table 0.3. (Values derived from Baseball-Reference.) Then

$$\rho_{BR} = (0.528, 0.197, 0.145, 0.048, 0.13, 0.068)$$

and

$$\rho_{TW} = (0.568, 0.212, 0.158, 0.054, 0.007, 0.054).$$

Using these probabilities in the script for Markov runs, the markov RPG for Babe Ruth is 12.65 and the value for Ted Williams is 12.55. The two values are close but Ruth has the slightly greater value.

No statistic can resolve the comparison between these two great players. Each played in different baseball eras, and each had particular strengths. Besides, what is to be the basis for comparison, their lifetime statistics used here, or the best career year for each? If the latter, how to choose the best career year? Note that Williams lost 3 (possibly best) years of his career to military service in World War II. It is interesting to compute the Markov runs for each, but the statistic won't answer this opinion question.

Chapter 9: Modeling Sports with Markov Chains.

9.1: Label the transient states in Figure 9.1 from 1 for 0:0 from to bottom, left to right and label the absorbing states last. Then 0:0 is state 1, state 40:30 is state 13, state 30:40 is state 15. The absorbing state "A wins" is 17 and "B wins" is 16. Use the script with this labeling.

For  $p = 0.6$ , the probability A wins is 0.736. For  $p = 0.6$ , the expected number of serves or points until absorption, that is the game ends, is 6.48 with a standard deviation of 2.59.

For  $p = 0.51$ , the probability A wins is 0.525. For  $p = 0.51$ , the expected number of serves or points until absorption, that is the game ends, is 6.75, only slightly longer. The standard deviation is 2.77, also slightly more.

The conclusion is that most games last between 4 and 9 serves, even if the players are nearly evenly matched. This makes sense, the game reaches the bottom row in 4 to 6 steps in any case and then is in the absorbing walk for a few steps.

9.2: Using a program script,

```
Mean A Scores:  90.14 Standard Deviation:  6.71
Mean B Scores: 100.64 Standard Deviation:  7.15
```

Chapter 10: Markov Chain Epidemic Models.

10.1: There is 1 state with  $S_t + I_t = 0$ , and 2 states with  $S_t + I_t = 1$ , namely  $S_t = 1$  with  $I_t = 0$  and  $S_t = 0$  with  $I_t = 1$ . Likewise there are  $i + 1$  states with  $S_t + I_t = i$  up to  $i = N$ . Then there are  $1 + 2 + \cdots + N + 1 = (N + 1)(N + 2)/2$  possible states.

10.2: The following script is a simple implementation of an epidemic on a two-dimensional grid. For a given value of  $N$ , the script defines a population of Susceptibles on a square grid of size  $2N + 1$ , and sets an Infective at the center location  $(N, N)$ . The infective can infect neighbors with probability  $p$ , and fails to infect neighbors with probability  $1 - p$ . Because the infection can only spread to immediate neighbors, the epidemic spreads through concentric rings of squares outward from the center. The spread in concentric rings means that the epidemic will take place over  $N$  steps, possibly stopping at some earlier step due to no Infectives, which the script reports. At each step, for all Infectives in the grid, the script successively infects immediate neighbors to the north, east, west and south with probability  $p$ . After possibly infecting neighbors, the infective becomes a Removed individual, so the infectious period lasts one step. At the end of each step, the script records the state of the epidemic. For testing and debugging, a value of  $N = 3$  is convenient. For an experiment, a value of  $N = 25$  is useful.

```

195 N <- 25
196 # N <- 3
197 p <- 0.6
198
199 popn <- matrix("S", 2*N+1, 2*N+1)
200 popn[N+1,N+1] <- "I"
201
202 dir <- list("N" = -1, "E" = 2*N+1, "S" = 1, "W" =
      -(2*N+1))
203
204 infect <- function(pos, d) {
205   if (popn[pos + d] == "S") {
206     if (runif(1) < p ){ popn[pos + d] <- "I"}
207   }
208 }
209
210 epidemic <- array("", dim=c(2*N+1, 2*N+1, N))
211
212 for (t in 1:N) { # RINGS or EPOCHS
213
214   infs <- which(popn == "I")
215   if (length(infs) == 0) {
216     cat("Epidemic ended after", t-1, "steps.\n")
217     break}
218   else {
219     for (j in infs) {
220       for (d in dir) {
221         infect(j, d)
222       }
223       popn[j] <- "R"
224     }
225     epidemic[, , t] <- popn
226   }
227 }
228
229 # # Animation code is adapted from
230 # # https://ryouready.wordpress.com/2010/11/21/
231 # # animate-gif-images-in-r-imagemagick/
232 # epidemicfactors <- array(as.numeric(factor(epidemic
233 #   )), dim=c(2*N+1, 2*N+1, N))
234 # par(xaxt="n", yaxt="n") #remove axis labels
235 #   and ticks
236 # png(file="epidemicImage%02d.png")
237 # for (t in 1:N) {
238 #   image(epidemicfactors[ , , t], col=c( "red", "
239 #     blue", "green" ))

```

```

236 # }
237 # dev.off()
238 # system("convert -delay 80 *.png epidemicAnimation.
      gif")
239
240 # file.remove(list.files(pattern=".png"))
      . language=R

```

This script is a very simple epidemic model with only basic attempts at efficiency. Many modifications are possible.

The animation is simple, relying on the graphics manipulation tool ImageMagick. The animation code is commented out because of the reliance on system dependent features. More elaborate animations are possible with other R packages such as plotly and gganimate.

Chapter 11: Reversible Markov Chains.

11.1: There are 6 detailed balance equations to check:

$$\begin{aligned}
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{1}{5} \cdot \frac{1}{2} \\
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{1}{5} \cdot \frac{1}{2} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{1}{5} \cdot \frac{1}{2} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{2}{5} \cdot \frac{1}{4} \\
 \frac{2}{5} \cdot \frac{1}{4} &= \frac{1}{5} \cdot \frac{1}{2}
 \end{aligned}$$

All are true, so the chain is reversible. Actually, only the first 3 equations need to be checked, since the last three are just the first three reversed.

11.2: Use the detailed balance to obtain  $\pi_1 P_{14} = \pi_4 P_{41}$  and  $\pi_1 P_{13} = \pi_3 P_{31}$  and  $\pi_3 P_{32} = \pi_2 P_{23}$  so  $\pi_1(1/2) = \pi_4(1/2)$  and  $\pi_1(3/40) = \pi_3(3/10)$  and  $\pi_3(1/4) = \pi_2(1/4)$ . Hence  $\pi_2 = \pi_3 = \pi_1/4 = \pi_4/4$ . Since the sum of the probabilities is 1,  $\pi_1 = \pi_4 = 4/10 = 2/5$  and  $\pi_2 = \pi_3 = 1/10$ .

11.3: This Markov chain has a stationary distribution

$$\pi = \left( \frac{1}{11}, \frac{4}{33}, \frac{1}{11}, \frac{4}{33}, \frac{5}{33}, \frac{4}{33}, \frac{1}{11}, \frac{4}{33}, \frac{1}{11} \right).$$

11.4: (a) The king makes a random walk on a graph with 32 vertices (the black squares) with degrees 1 on 2 corner squares, 2 on 12 side squares, and 4 on 18 interior squares. For a corner square  $i$ ,  $\pi_i = \frac{1}{1 \cdot 2 + 2 \cdot 12 + 4 \cdot 18} = \frac{1}{98}$  so the answer is 98.

(b) Label one corner starting square as state 1 and the other corner starting square as state 32. The stationary probability of occupying state 1 is  $\pi_1 = \frac{1}{98}$  and the stationary probability of occupying state 32 is also  $\pi_1 = \frac{1}{98}$ . Since the walks are independent processes, the joint probability of

occupying both states simultaneously is  $\pi_1\pi_{32} = \frac{1}{98^2}$  and the expected number of steps is  $98^2$ .

11.5: For general  $n \geq 5$ , it is necessary to check each loop of length 3, of which there are  $\binom{n}{3}$ , and once those 3 states chosen, there is only one way to write the criterion equation. Then the number of 3 state loops can be written as  $\binom{n}{3}(3-1)!/2$ .

For the loops over 4 states, there are  $\binom{n}{4}$  choices of states. For the chosen set of 4, fix the starting state and there are  $3!$  orders for the remaining states. However, since the other side of the equation is the reversed path, there are only  $3!/2$  distinct paths of 4 states with the first state fixed.

For the loops over 5 states, there are  $\binom{n}{5}$  choices of states. For the chosen set of 5, fix the starting state and there are  $4!$  orders for the remaining states. However, since the other side of the equation is the reversed path, there are only  $4!/2$  distinct paths of 5 states with the first state fixed.

The same argument continues for general  $n \geq 5$ .

11.6: Suppose the Markov chain has a state  $j_{(*)}$  with  $P_{ij_{(*)}} > 0$  and  $P_{j_{(*)}i} > 0$  for  $1 < i < k$ . The goal is to show the Markov chain is reversible if and only if

$$P_{j_{(*)},j_1}P_{j_1,j_2}P_{j_2,j_{(*)}} = P_{j_{(*)},j_2}P_{j_2,j_1}P_{j_1,j_{(*)}}$$

for all  $1 < j_1, j_2 < k$ . Then

$$P_{j_1j_2} = \frac{P_{j_{(*)}j_2}}{P_{j_{(*)}j_1}}P_{j_2j_1}\frac{P_{j_1j_{(*)}}}{P_{j_2j_{(*)}}}.$$

This rewritten equality uses the hypothesis that  $P_{ij_{(*)}} > 0$  and  $P_{j_{(*)}i} > 0$ . Start with the loop probability

$$P_{j_0j_1}P_{j_1j_2}\cdots P_{j_{\ell-1}j_\ell}P_{j_\ell j_0}$$

and substitute the rewritten three step equality to obtain

$$\frac{P_{j_{(*)}j_1}}{P_{j_{(*)}j_0}}P_{j_1j_0}\frac{P_{j_0j_{(*)}}}{P_{j_1j_{(*)}}}\frac{P_{j_{(*)}j_2}}{P_{j_{(*)}j_1}}P_{j_2j_1}\frac{P_{j_1j_{(*)}}}{P_{j_2j_{(*)}}}\cdots\frac{P_{j_{(*)}j_\ell}}{P_{j_{(*)}j_{\ell-1}}}P_{j_\ell j_{\ell-1}}\frac{P_{j_{\ell-1}j_{(*)}}}{P_{j_\ell j_{(*)}}}\frac{P_{j_{(*)}j_0}}{P_{j_{(*)}j_\ell}}P_{j_0j_\ell}\frac{P_{j_\ell j_{(*)}}}{P_{j_0j_{(*)}}}.$$

Many terms cancel in a telescoping fashion, and reversing the order of multiplication gives the right side of the Kolmogorov loop criterion.

Brill et al. say Kelly *Reversibility and Stochastic Networks*, 1978, Cambridge University Press, Exercise 1.5.2, says that if there is a state which can be accessed *from* every other state in exactly 1 step, i.e. a column of the transition matrix has nonzero entries, then it is sufficient to check loops of only 3 states. However, neither source provides the proof, so it is possible that the exercise is mistaken. No counterexample is provided here, so the less restrictive criterion remains open here.

Chapter 12: Lumped Markov Chains.

12.1: To conform to the theorem, reorder the states to  $s_1, s_5, s_2, s_4, s_3$  so

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

Since this is an absorbing, not an irreducible and aperiodic, chain, applying the observation that all that is needed for  $U$  is that the  $i$ th row should be a probability vector with nonzero components only for states in  $E_i$

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

and

$$V = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then

$$VUPV = PV = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ 1/2 & 0 & 1/2 \\ 0 & 10 & 0 \end{pmatrix}$$

so the absorbing random walk is lumpable.

First calculate all the quantities for the original random walk.

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

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

$$N = (I_3 - Q)^{-1} = \begin{pmatrix} 3/2 & 1/2 & 1 \\ 1/2 & 3/2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

$$\mathbf{w} = N\mathbf{1} = (3, 3, 4)^T$$

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

Next calculate the absorption quantities for the lumped chain from the original chain using the submatrices  $U_A, U_T, V_A, V_T$  of  $U, V$ .

$$\begin{aligned}\hat{P} &= \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \end{pmatrix}, \\ \hat{N} &= U_T N V_T = \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix}, \\ \hat{\mathbf{w}} \hat{N} \mathbf{1} &= (3, 4)^T, \\ \hat{B} &= U_T B V_A = (1, 1)^T.\end{aligned}$$

Finally calculate the absorption quantities from the lumped chain canonical  $\hat{P}$  directly.

$$\begin{aligned}\hat{Q} &= \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \end{pmatrix}, \hat{R} = (1/2, 0)^T, \\ \hat{N} &= (I_T - \hat{Q})^{-1} = \begin{pmatrix} 2 & 1 \\ 2 & 2 \end{pmatrix}, \\ \hat{\mathbf{w}} &= \hat{N} \mathbf{1} = (3, 4)^T, \\ \hat{B} &= \hat{N} \hat{R} = (1, 1)^T.\end{aligned}$$

Both calculations of the absorption quantities agree.

12.2: On the left side

$$U_{ij} = \begin{cases} \pi_j / \sum_{x_\nu \in E_i} \pi_\nu & x_j \in E_i \\ 0 & \text{otherwise.} \end{cases}$$

On the right side,  $V_{ji} = 1$  if  $x_j \in E_i$  and 0 otherwise. Because  $\hat{\pi} = \pi V$ ,  $\hat{\pi}_i = \sum_{x_\nu \in E_i} \pi_\nu$ . Then the terms on the right side correspond precisely to the terms on the left side.

12.3: As a weighted random walk on a graph, the lazy random walk as a Markov chain is irreducible and reversible. For a hypercube of dimension  $k$ , the number of edges from each vertex is the dimension of the hypercube  $k$ , and the total number of vertices is  $2^k$ . The lazy random walk is associated with the weighted graph with self-edges with weight  $w_{ii} = k$  and  $k$  edges each with weight  $w_{ij} = 1$ . The sum of all weights from the  $2^k$  nodes is

$$s = \sum_{i,j} w_{ij} = (2k) \cdot 2^k.$$

The section on Reversible Markov Chains shows the invariant distribution is

$$\pi_i = \frac{2k}{(2k) \cdot 2^n} = \frac{1}{2^n}.$$

12.4: Entry  $i$  must satisfy

$$\binom{k}{i-1} \left(\frac{1}{2}\right)^k \cdot \frac{k-i+1}{2k} + \binom{k}{i} \left(\frac{1}{2}\right)^k \cdot \frac{1}{2} + \binom{k}{i+1} \left(\frac{1}{2}\right)^k \cdot \frac{i+1}{2k} = \binom{k}{i} \left(\frac{1}{2}\right)^k$$

or more simply

$$\binom{k}{i-1} \cdot \frac{k-i+1}{2k} + \binom{k}{i} \cdot \frac{1}{2} + \binom{k}{i+1} \cdot \frac{i+1}{2k} = \binom{k}{i}.$$

This reduces to

$$\binom{k-1}{i-1} + \binom{k-1}{i+1} = \binom{k}{i},$$

the basic binomial (Pascal triangle) identity.

12.5: For lumpability, check that for every pair of sets  $E_\xi$  and  $E_\eta$ ,  $\sum_{x_\nu \in E_\eta} p_{i\nu}$  has the same value for every  $x_i \in E_\xi$ . These common values form the transition probabilities  $\hat{p}_{\xi,\eta}$  for the lumped chain. If  $\xi$  and  $\eta$  differ by more than 1, then for every  $x_i \in E_\xi$ ,  $p_{i,\nu} = 0$  for  $\nu \in E_\eta$ , so  $\sum_{x_\nu \in E_\eta} p_{i\nu} = 0$ . If  $\xi - \eta = 1$  then for every  $x_i \in E_\xi$ ,  $p_{i,\nu} = \frac{1}{n}$  and  $\sum_{x_\nu \in E_\eta} p_{i\nu} = \frac{\xi}{n}$ . If  $\xi - \eta = -1$  then for every  $x_i \in E_\xi$ ,  $p_{i,\nu} = \frac{1}{n}$  and  $\sum_{x_\nu \in E_\eta} p_{i\nu} = \frac{n-\xi}{n}$ . This proves the lumpability criterion.

12.6:

$$P = \begin{matrix} & \begin{matrix} 000 & 100 & 010 & 001 & 101 & 011 & 110 & 111 \end{matrix} \\ \begin{matrix} 000 \\ 100 \\ 010 \\ 001 \\ 101 \\ 011 \\ 110 \\ 111 \end{matrix} & \begin{pmatrix} 1/2 & 1/6 & 1/6 & 1/6 & 0 & 0 & 0 & 0 \\ 1/6 & 1/2 & 0 & 0 & 1/6 & 0 & 1/6 & 0 \\ 1/6 & 0 & 1/2 & 0 & 0 & 1/6 & 1/6 & 0 \\ 1/6 & 0 & 0 & 1/2 & 1/6 & 1/6 & 0 & 0 \\ 0 & 1/6 & 0 & 1/6 & 1/2 & 0 & 0 & 1/6 \\ 0 & 0 & 1/6 & 1/6 & 0 & 1/2 & 0 & 1/6 \\ 0 & 1/6 & 1/6 & 0 & 0 & 0 & 1/2 & 1/6 \\ 0 & 0 & 0 & 0 & 1/6 & 1/6 & 1/6 & 1/2 \end{pmatrix} \end{matrix}.$$

The transition probability matrix is symmetric so the random walk Markov chain is reversible with stationary vector previously determined to be

$$\boldsymbol{\pi} = (1/8, 1/8, 1/8, 1/8, 1/8, 1/8, 1/8, 1/8).$$

The eigenvalues of  $P$  are  $1, 2/3, 1/3, 0$  with multiplicities  $1, 3, 3, 1$  respectively, so  $\lambda_2 = 2/3$ .

The partition is

$$\hat{S} = \{E_0, E_1, E_2, E_3\} = \{\{000\}, \{100, 010, 001\}, \{101, 011, 110\}, \{111\}\}.$$

The lumped transition probability matrix is

$$\hat{P} = \begin{matrix} & \begin{matrix} E_0 & E_1 & E_2 & E_3 \end{matrix} \\ \begin{matrix} E_0 \\ E_1 \\ E_2 \\ E_3 \end{matrix} & \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/6 & 1/2 & 2/6 & 0 \\ 0 & 2/6 & 1/2 & 1/6 \\ 0 & 0 & 1/2 & 1/2 \end{pmatrix} \end{matrix}$$



with  $\hat{\pi} = (1/8, 3/8, 3/8, 1/8)$ .

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$V = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$VUP = \begin{pmatrix} 1/2 & 1/6 & 1/6 & 1/6 & 0 & 0 & 0 & 0 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/9 & 1/9 & 1/9 & 0 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/9 & 1/9 & 1/9 & 0 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/9 & 1/9 & 1/9 & 0 \\ 0 & 1/9 & 1/9 & 1/9 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0 & 1/9 & 1/9 & 1/9 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0 & 1/9 & 1/9 & 1/9 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0 & 0 & 0 & 0 & 1/6 & 1/6 & 1/6 & 1/2 \end{pmatrix}.$$

Because the stationary distribution is uniform, the  $\pi$ -norm is simply scaling the standard Euclidean norm by  $\sqrt{8}$ . Then use the following R script.

```

1      # Enter matrices by rows, so use keyword byrow
2      P <- matrix( c(1/2,
3                    1/6, 1/6, 1/6, 0, 0, 0, 0, 1/6, 1/2, 0, 0, 1/
4                    6, 0, 1/6, 0, 1/6,
5                    0, 1/2, 0, 0, 1/6, 1/6, 0, 1/6, 0, 0, 1/2, 1/
6                    6, 1/6, 0, 0, 0,
7                    1/6, 0, 1/6, 1/2, 0, 0, 1/6, 0, 0, 1/6, 1/6,
8                    0, 1/2, 0, 1/6, 0,
9                    1/6, 1/6, 0, 0, 0, 1/2, 1/6, 0, 0, 0, 0, 1/6,
10                   1/6, 1/6, 1/2),
11                byrow=TRUE, nrow=8, ncol=8)
12
13     V <- matrix( c(1, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0,
14                   0, 0, 1, 0, 0,
15                   0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0,
16                   1), byrow=TRUE,
17                 nrow=8, ncol=4)
18
19     U <- matrix( c(1, 0, 0, 0, 0, 0, 0, 0, 0, 1/3,
20                   1/3, 1/3, 0, 0,
```

```

14      0, 0, 0, 0, 0, 0, 1/3, 1/3, 1/3, 0, 0, 0, 0,
      0, 0, 0, 0, 1),
15      byrow=TRUE, nrow=4, ncol=8)
16
17      D <- diag(1/sqrt(8), nrow=8, ncol=8)
18      Dinverse <- diag(sqrt(8), nrow=8, ncol=8)
19
20      lambda2 <- 2/3
21
22      N <- 10
23      H <- V %*% U %*% P
24      Hn <- H
25      Pn <- P
26
27      normdifference <- c( norm( Dinverse %*% (Hn - Pn)
      %*% D, type="2") )
28      for (n in 1:(N-1)) {
29          Hn <- H %*% Hn
30          Pn <- P %*% Pn
31          normdifference <- c( normdifference, norm(
      Dinverse %*% (Hn - Pn) %*% D, type="2") )
32      }
33      plot(normdifference, col="blue")
34
35      K <- function(n, l2) { n * l2^{n-1} }
36      points(K(1:N, lambda2), col="red")
37

```

12.7: (1) For the lumped chain,

$$\|pV\|_{\hat{\pi}} = \sqrt{(1/12)^2/(1/5) + (11/12)^2/(4/5)} = \sqrt{625/576} \approx 1.042.$$

For the original chain

$$\|p\|_{\pi} = \sqrt{(1/6)^2/(2/5) + (1/12)^2/(1/5) + (3/4)^2/(2/5)} = \sqrt{145/96} \approx 1.229.$$

(2) The definitions of the respective norms are

$$\|pV\|_{\hat{\pi}} = \sqrt{\sum_{\nu} (pV)_{\nu}^2 / \hat{\pi}_{\nu}}.$$

and

$$\|p\|_{\pi} = \sqrt{\sum_{\nu} p_{\nu}^2 / \pi_{\nu}}$$

It suffices to show that for any  $E_{\xi}$  in the partition

$$\sum_{\nu \in E_{\xi}} (p_{\nu})^2 / \pi_{\xi} \leq \sum_{\nu \in E_{\xi}} p_{\nu}^2 / \pi_{\nu}.$$

At first glance, this appears to be an application of a variant of the Cauchy-Schwarz Inequality or Jensen's Inequality. However, the inequality is not in the right form for either.

First take the case with 2 components  $x_1$  and  $x_2$  in  $E_\xi$  and consider the expression in the form

$$\frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} - \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} = \frac{\pi_2 x_1^2 - 2\pi_1 \pi_2 x_1 x_2 + \pi_1 x_2^2}{\pi_1 \pi_2 (\pi_1 + \pi_2)} = \frac{(\pi_2 x_1 - \pi_1 x_2)^2}{\pi_1 \pi_2 (\pi_1 + \pi_2)} \geq 0$$

so the expression is positive semi-definite, as expected. Note that the expression is 0 along the line  $(\pi_1 t, \pi_2 t)$ .

Next take the case with 3 components  $x_1, x_2$  and  $x_3$  in  $E_\xi$ .

$$\begin{aligned} \frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} + \frac{x_3^2}{\pi_3} - \frac{(x_1 + x_2 + x_3)^2}{\pi_1 + \pi_2 + \pi_3} = \\ \frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} - \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} + \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} + \frac{x_3^2}{\pi_3} - \frac{(x_1 + x_2 + x_3)^2}{\pi_1 + \pi_2 + \pi_3}. \end{aligned}$$

The two-component expression

$$\frac{x_1^2}{\pi_1} + \frac{x_2^2}{\pi_2} - \frac{(x_1 + x_2)^2}{\pi_1 + \pi_2}$$

is nonnegative as shown above. Then consider

$$\frac{(x_1 + x_2)^2}{\pi_1 + \pi_2} + \frac{x_3^2}{\pi_3} - \frac{(x_1 + x_2 + x_3)^2}{\pi_1 + \pi_2 + \pi_3}.$$

as a similar two-component solution say with  $u_1 = (x_1 + x_2)$ ,  $u_2 = x_3$ ,  $\rho_1 = (\pi_1 + \pi_2)$  and  $\rho_2 = \pi_3$ . Then it too will be nonnegative, and the original three-component expression will be positive semidefinite. Note that the three-component expression is 0 along the line  $(\pi_1 t, \pi_2 t, \pi_3 t)$ .

Continue this process inductively until the entire original expression is shown to be nonnegative and the inequality holds.

12.8:

$$\begin{aligned} \|x_0 V \hat{P}^n - x_0 P^n V\|_{\hat{\pi}} &= \|x_0 V U P^n V - x_0 P^n V\|_{\hat{\pi}} \\ &= \|(x_0 V U P^n - x_0 P^n) V\|_{\hat{\pi}} \\ &\leq \|(x_0 V U P^n - x_0 P^n)\|_{\pi} \\ &\leq \|x_0\| \cdot \|V U P^n - P^n\|_{\pi} \\ &\leq \|x_0\| \cdot K(n) \cdot \delta \leq \|x_0\| \cdot n \cdot |\lambda_2|^{n-1} \cdot \delta. \end{aligned}$$

1: If  $\sigma = [123]$  and the transposition is  $(1, 2)$ , then  $\sigma^* = (1, 2)[123] = [213]$ , with  $d(\sigma^*, \sigma_0) = 1$  while  $d(\sigma, \sigma_0) = 0$ . The second case applies and the transition probability  $P([123], [213]) = \theta/3$ . Similar calculations apply for  $(1, 3)$  with  $\sigma^* = [321]$  and  $(2, 3)$  with  $\sigma^* = [132]$ . This is enough information to fill the first row of the transition probability matrix.

If  $\sigma = [132]$  and the transposition is  $(1, 2)$ , then  $\sigma^* = (1, 2)[132] = [231]$ , with  $d(\sigma^*, \sigma_0) = 2$  while  $d(\sigma, \sigma_0) = 1$ . The second case applies and the transition probability  $P([132], [231]) = \theta/3$ . If  $\sigma = [132]$  and the transposition is  $(1, 3)$ , then  $\sigma^* = (1, 3)[132] = [312]$ , with  $d(\sigma^*, \sigma_0) = 2$  while  $d(\sigma, \sigma_0) = 1$ . The second case applies again and the transition probability  $P([132], [312]) = \theta/3$ .

If  $\sigma = [132]$  and the transposition is  $(2, 3)$ , then  $\sigma^* = (2, 3)[132] = [123]$ , with  $d(\sigma^*, \sigma_0) = 0$  while  $d(\sigma, \sigma_0) = 1$ . The first case applies again and the transition probability  $P([132], [123]) = 1/3$ . Similar calculations apply for  $(1, 3)$  with  $\sigma^* = [312]$  and  $(2, 3)$  with  $\sigma^* = [132]$ . This enough information to complete the fourth row of the transition probability matrix.

If  $\sigma = [312]$  and the transposition is  $(1, 2)$ , then  $\sigma^* = (1, 2)[312] = [321]$ , with  $d(\sigma^*, \sigma_0) = 1$  while  $d(\sigma, \sigma_0) = 2$ . The first case applies and the transition probability  $P([312], [321]) = 1/3$ . Similar calculations apply for  $(1, 3)$  with  $\sigma^* = [132]$  and  $(2, 3)$  with  $\sigma^* = [213]$ .

The other rows are similar.

2: For  $\theta = 1/2$ ,  $P^{10}$  is (to three decimal places)

$$\begin{pmatrix} 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.333 & 0.167 & 0.167 & 0.167 & 0.083 & 0.083 \\ 0.334 & 0.166 & 0.166 & 0.166 & 0.084 & 0.084 \\ 0.334 & 0.166 & 0.166 & 0.166 & 0.084 & 0.084 \end{pmatrix}$$

agreeing with the stationary distribution.

3: The algorithm needs to shuffle an array in a way such that all  $n!$  permutations are equally likely. One important property of the  $n!$  permutations is that any given position (say  $j$ ) will be populated by a given element (say  $i$ ) with probability  $1/n$ . This is because, out of the  $n!$  permutations,  $(n-1)!$  contain element  $j$  at location  $i$ . Due to this equidistribution, we can try to first fix the element at a particular (in this case, the last) location and then process the remaining elements. The first step of the algorithm guarantees the probability of the last entry being  $j$  is  $1/n$ , the second step of the algorithm guarantees the probability of the second-last entry being  $j$  is  $1/(n-1)$  and so on. Inductively then, the probability of a given permutation is  $1/n!$ .

1: Case 1: Suppose  $x'$  is chosen according to  $P(x, x')$  with  $x \neq x'$  and

$$A(x, x') = \frac{\pi(x')P(x', x)}{\pi(x)P(x, x')} \geq 1.$$

Then  $Q(x, x') = P(x, x')$  so the left side becomes  $\pi(x)Q(x, x') = \pi P(x, x')$ . On the right hand side, since  $A(x, x') \geq 1$ , then

$$A(x', x) = \frac{\pi(x)P(x, x')}{\pi(x')P(x', x)} \leq 1.$$

so

$$Q(x', x) = P(x', x)A(x', x) = P(x', x) \frac{\pi(x)P(x, x')}{\pi(x')P(x', x)}.$$

so  $\pi(x)Q(x', x) = \pi(x)P(x, x')$ .

Case 2: Case 1: Suppose  $x'$  is chosen according to  $P(x, x')$  with  $x \neq x'$  and

$$A(x, x') = \frac{\pi(x')P(x', x)}{\pi(x)P(x, x')} < 1.$$

is similar.

- 2: (a) For  $N = 3$ , the transition probability matrix is

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/9 & 4/9 & 4/9 & 0 \\ 0 & 4/9 & 4/9 & 1/9 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

- (b) The stationary distribution is  $\pi = (1/20, 9/20, 9/20, 1/20)$ .  
 (c) For simplicity and without prior knowledge on the transitions among the 4 states choose

$$\begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{pmatrix}.$$

Then the denominator of the  $\alpha_{ij}$  values is

$$\alpha_{ij} = \frac{1}{1 + \frac{\pi_i p_{ij}}{\pi_j p_{ji}}} = \frac{1}{1 + \frac{\pi_i}{\pi_j}}.$$

The matrix of  $\alpha_{ij}$  values is

$$\begin{pmatrix} \frac{1}{2} & \frac{9}{10} & \frac{9}{10} & \frac{1}{2} \\ \frac{1}{10} & \frac{1}{2} & \frac{1}{2} & \frac{1}{10} \\ \frac{1}{10} & \frac{9}{2} & \frac{9}{10} & \frac{1}{10} \\ \frac{1}{2} & \frac{1}{10} & \frac{1}{10} & \frac{1}{2} \end{pmatrix}.$$

Since all entries are between 0 and 1, choose  $s_{ij} = 1$ . Then the matrix  $Q$  for the Metropolis-Hastings algorithm is

$$\begin{pmatrix} \frac{17}{40} & \frac{9}{40} & \frac{9}{40} & \frac{1}{8} \\ \frac{1}{40} & \frac{33}{40} & \frac{1}{40} & \frac{1}{40} \\ \frac{1}{40} & \frac{1}{40} & \frac{33}{40} & \frac{1}{40} \\ \frac{1}{40} & \frac{9}{8} & \frac{9}{40} & \frac{17}{40} \end{pmatrix}.$$

This has the same stationary distribution.

- (d) The eigenvalues of  $P$  are  $1, 1/3, -1/9, -1/3$ . The rate of convergence to the stationary distribution is approximately  $(1/3)^n$ .  
 (e) The eigenvalues of  $Q$  are  $1, 7/10, 1/2, 3/10$ . The rate of convergence to the stationary distribution is approximately  $(7/10)^n$ , much slower.
- 3: (a) Since each state has a positive probability of transitioning to its neighbor state, the chain is irreducible. Alternatively, each entry in  $P^4$  is non-zero, so the chain is irreducible. Since this is a finite state space irreducible chain, it is positive recurrent. Since each state has a positive probability of staying in the state, the minimum return time is 1, so the chain is aperiodic.
- (b)

$$\pi = \left( \frac{1}{16}, \frac{1}{4}, \frac{3}{8}, \frac{1}{4}, \frac{1}{16} \right).$$

- (c) It is easy to check the reversibility, but both the physical description, and the symmetry of  $\pi$  and  $P$  suggest that reversibility holds.  
 (d) The eigenvalues, ordered by decreasing value, are  $1, 3/4, 1/2, 1/4, 0$ .

(e) The corresponding eigenvectors, without normalization, are

$$(1, 1, 1, 1, 1)^T, (1, 1/2, 0, -1/2, -1)^T, (1, 0, -1/3, 0, 1)^T, \\ (1, -1/2, 0, 1/2, -1)^T, (1, -1, 1, -1, 1)^T.$$

(f) The weighted inner products of each eigenvector with itself is respectively  $1, 1/4, 1/6, 1/4, 1$  so the normalized eigenvectors are

$$(1, 1, 1, 1, 1)^T, (2, 1, 0, -1, -2)^T, \left(\sqrt{6}, 0, -\frac{\sqrt{6}}{3}, 0, \sqrt{6}\right)^T, \\ (2, -1, 0, 1, -2)^T, (1, -1, 1, -1, 1)^T.$$

(g) With (for example) the Maxima command

```
generateP: genmatrix(lambda([i,j], pi[j] *
sum(lambda[k]*psi[k][i]*psi[k][j], k, 1, 5)[1]), 5, 5);
the result is
```

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{8} & \frac{1}{4} & \frac{3}{8} & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\ 0 & 0 & \frac{3}{8} & \frac{1}{2} & \frac{1}{8} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

as expected.

- 4: (a) Using the normalized eigenvectors from the previous solution, the upper bound is:

$$\frac{1}{4} \sum_{i=2}^{\text{card}(\mathcal{X})} \lambda_i^{2n} \psi_i(x)^2 \\ = \frac{1}{4} \left[ \left(\frac{3}{4}\right)^{2n} \cdot (-2)^2 + \left(\frac{1}{2}\right)^{2n} \cdot (\sqrt{6})^2 + \left(\frac{1}{4}\right)^{2n} \cdot (-2)^2 + (0)^{2n} \cdot (-2)^2 \right] \\ = \left(\frac{3}{4}\right)^{2n} + \frac{3}{2} \cdot \left(\frac{1}{2}\right)^{2n} + \left(\frac{1}{4}\right)^{2n}$$

- (b) After 5 steps, the total variation distance squared is approximately 0.0359 and the upper bound is approximately 0.0578 so the inequality bound holds. After 10 steps, the total variation distance squared is approximately 0.00181 and the upper bound is approximately 0.00317 so the inequality bound holds.

5:

$$\begin{aligned}
\langle Pg, h \rangle &= \sum_x \sum_y P(x, y) g(y) h(x) \pi(x) \\
&= \sum_x \sum_y g(y) h(x) \pi(x) P(x, y) \\
&= \sum_x \sum_y g(y) h(x) \pi(y) P(y, x) \\
&= \sum_x \sum_y g(y) P(y, x) h(x) \pi(y) \\
&= \sum_y \sum_x g(y) P(y, x) h(x) \pi(y) \\
&= \sum_y g(y) \sum_x P(y, x) h(x) \pi(y) \\
&= \langle g, Ph \rangle.
\end{aligned}$$

6: Let  $\mathbf{e}_x$  be the elementary column vector with 1 at position  $x$  and 0 elsewhere.

Since  $\mathbf{e}_x$  is a probability distribution concentrated entirely on state  $x$ , then  $\mathbf{e}_x^T \cdot P$  is the probability distribution of states after one step from  $x$ . Then  $\mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y$  picks out  $P(x, y)$ , that is,  $\mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y = P(x, y)$ . The point is that this probability product does not involve the inner product weight vector  $\pi$ .

The orthonormal eigenvector basis represents  $\mathbf{e}_x$  in terms of  $\psi_i$  as  $\mathbf{e}_x = \sum_i a_{xi} \psi_i$  for some scalars  $a_{xi}$ . Projecting  $\mathbf{e}_x$  against  $\psi_i$  with the weighted inner product

$$a_{xi} = \langle \mathbf{e}_x, \psi_i \rangle = \psi_i(x) \pi(x)$$

so as a column vector

$$\mathbf{e}_x = \sum_i \psi_i(x) \pi(x) \psi_i.$$

Using

$$P(x, y) = \mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y$$

where  $\mathbf{e}_x^T \cdot P \cdot \mathbf{e}_y$  indicates the usual matrix-vector product with rows dotted against columns, and expressing  $\mathbf{e}_y$ , but not  $\mathbf{e}_x$ , in terms of the orthonormal basis

$$\begin{aligned}
&= \mathbf{e}_x \cdot P \cdot \left( \sum_i \psi_i(y) \pi(y) \psi_i \right) \\
&= \mathbf{e}_x \cdot \left( \sum_i \psi_i(y) \pi(y) P \cdot \psi_i \right) \\
&= \mathbf{e}_x \cdot \left( \sum_i \psi_i(y) \pi(y) \lambda_i \psi_i \right)
\end{aligned}$$

using the eigenvector property. Now factoring the dot product with  $\mathbf{e}_x$  through the sum will pick out the  $x$ th term from each  $\psi_i$ ,

$$\begin{aligned} &= \sum_i \psi_i(y) \pi(y) \lambda_i (\mathbf{e}_x \cdot \psi_i) \\ &= \sum_i \psi_i(y) \pi(y) \lambda_i \psi_i(x) \end{aligned}$$

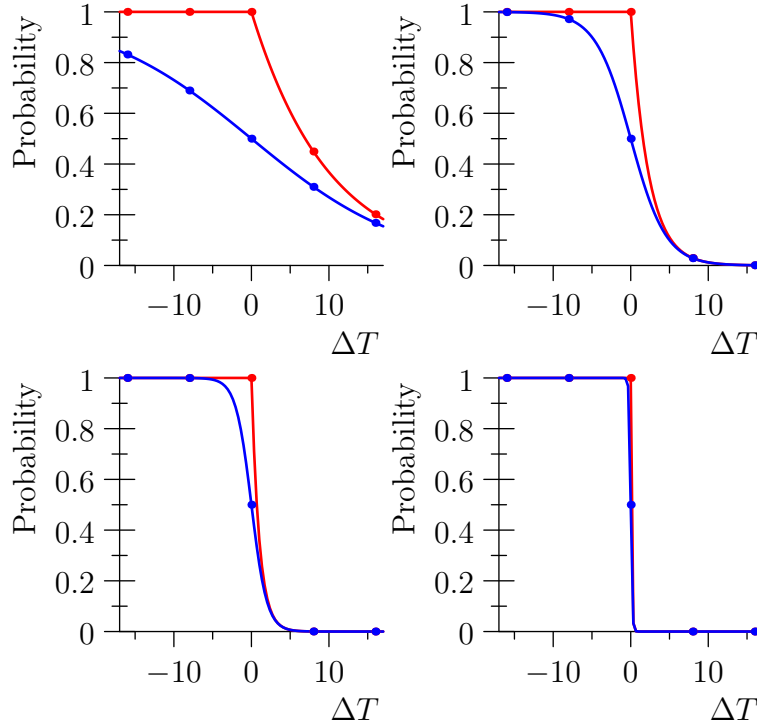
and finally,  $\pi(y)$  is independent of the summation over  $i$  so it can be factored out of the sum, and rearranging the products yields

$$= \pi(y) \sum_i \lambda_i \psi_i(x) \psi_i(y).$$

- 1: With  $n$  sites, the chance of missing a site is  $1 - \frac{1}{n}$ . In  $n$  iterations of the selection, the chance of missing the site is  $(1 - \frac{1}{n})^n \approx 1/e$  for  $n$  large. Among  $n$  sites there will be approximately  $1/e \cdot n$  sites missed.
- 2:

$$\Delta E = E(\omega') - E(\omega) = -2J(\omega'_{(i,j)} - \omega_{(i,j)}) \sum_{k=1}^4 \omega_{\langle i,j \rangle [k]}$$

where the sum is only over the four nearest neighbors of the  $(i, j)$  site. The difference  $(\omega'_{(i,j)} - \omega_{(i,j)}) = \pm 2$ . The sum over the four nearest neighbors will be  $\pm 4$  if all 4 neighbors have the same sign,  $\pm 2$  if 3 neighbors have the same sign, and 0 if 2 are opposite, and 1 is opposite, and 0 if 2 of the neighbors have one sign, and the other 2 are opposite. Then  $\Delta E$  can only have the values  $-16, -8, 0, +8, +16$ .



3:



4: For the Metropolis chains with the deterministic visitation rule, consider configuration  $\omega$  and configuration  $\omega'$  which differs in one site. It is possible to go from  $\omega$  to  $\omega'$  in at most  $N^2$  steps, each of which has non-zero probability (although it may be small!) of occurring. That is, all configurations communicate, and the chain is irreducible.

The same argument holds for the Glauber chain with the random selection visitation rule, although the expected time to reach one state from another is longer as in the coupon collectors problem, and the probability of movement is smaller.

5: An important feature of the puzzle is that all fleas move independently. The problem has two challenges:

- not all squares on a grid are created equal since edge squares have fewer neighbors than interior squares, and
- the process lasts for only 50 periods, so without further investigation, it is not apparent how close it is to a stationary distribution.

The last item means that the solution will have to be computational.

To build an intuition, assume instead all squares are equal and that 50 can be considered a long period of time. Then a flea can be in one of the  $30 \cdot 30 / 2 = 450$  squares with equal probability. Why 450 and not 900? To see this assume the grid was painted in black and white like a chessboard. After 50 moves a flea starting on a white square must be on a white square; similarly a flea starting on a black square must be on a black square. This is similar to the reasoning in 1-dimensional random walk that after an even number of steps, the walker is at an even-numbered position.

What is the probability that some given square is empty after 50 moves? There are 450 fleas that potentially independently can occupy it. (Notice that any flea can reach any square in no more than 60 jumps.) Therefore the probability that a square is *not* occupied by any flea is  $(1 - 1/450)^{450} \approx e^{-1} \approx 0.367470$ . Taking expectations over all 900 fleas, the number of empty squares will be  $900 \cdot (1 - 1/450)^{450} \approx 330.723$ .

However, the variance will be approximately  $e^{-1}(1 - e^{-1})/N \approx \frac{0.23254}{N}$ . To get the answer to six decimal places means the estimate will need to have at least  $\sqrt{\frac{0.23254}{N}} < 5 \times 10^{-7}$ , or at least  $N > 9.3 \times 10^{11}$  or more than  $900 \cdot 9.3 \times 10^{11} = 8.4 \times 10^{14}$  flea moves. Even with current modern processors working in parallel, simulation will take too long to achieve the desired accuracy.

Making 10,000 simulations of 50 steps each using the following script gives a mean value of 331.8646.

```

1 # set.seed(2023)                                #for testing,
   debugging
2 N <- 30
3 sims <- 10000
4
5 inbounds <- function(x) { all(x >= 1) && all(x <= N)
   }

```

```

6
7 # Denote the location of a flea by (i, j). Here is a
  function
8 # that gives us a _list_ of locations where a flea at
  (i,j) can jump.
9 # The key element of this function is removing
  potential locations that
10 # are out of bounds.
11 neighbors <- function(site) {
12   adjacencies <- list( c(1,0), c(-1,0), c(0, 1), c
     (0,-1) )
13   nbrs <- lapply(adjacencies, function(x) x + site)
14   realNbrs <- sapply(nbrs, inbounds)
15   nbrs[ realNbrs ]
16 }
17
18 # Create two helper
19 # functions that recode (i, j) position of a flea to
  its numeric index:
20 site2i <- function(site) {
21   site[1] + (site[2] - 1) * N
22 }
23
24 i2site <- function(i) {
25   s <- c( ( (i-1) %% N + 1 ), ((i-1) %% N + 1) )
26   return(s)
27 }
28
29 # Create a list, which in cell (i, j) recoded by
  site2i( (i,j) )
30 # stores the target locations for a flea:
31 NEI <- list()
32 for (i in 1:N) {
33   for (j in 1:N) {
34     s <- site2i( c(i,j) )
35     NEI[[s]] <- neighbors( c(i,j) )
36   }
37 }
38
39 # The idea of the simulation is to initialize it
  with N^2 fleas,
40 # each starting on a different square, recoded by
  site2i
41 fleas <- list()
42 for (i in 1:N) {
43   for (j in 1:N) {
44     s <- site2i( c(i,j) )

```

```

45     fleas[[s]] <- c(i,j)
46   }
47 }
48
49 result <- numeric(sims)
50
51 for (sim in 1:sims) {
52   # Then each flea on a square moves randomly to one of
53   # the locations it is allowed to occupy.
54   for (i in 1:N^2) {
55     f <- fleas[[i]]           #find
56     site flea is on now
57     s <- site2i(f)           #recode
58     to position in NEI
59     l <- length(NEI[[s]] )   #count
60     adjacent sites
61     r <- sample(1:l, 1)      #choose
62     one randomly
63     newSite <- NEI[[s]][[r]]  #fix
64     newSite as the chosen
65     fleas[[i]] <- newSite    #make
66     that new site for flea i
67   }
68
69   # Create a matrix to record unoccuied squares.
70   # Initially it will say all sites are unoccupied
71   # (with a 1 for TRUE).
72   unoccupied <- matrix(1, N, N)
73   # If a site is occupied after a jump, change to 0
74   # (FALSE).
75   for (i in 1:N^2) {
76     unoccupied[ i2site(fleas[[i]])[1], i2site(
77     fleas[[i]])[2] ] <- 0
78   }
79   result[sim] <- sum(unoccupied)
80 }
81
82 mean(result)

```

Using the following script, using floating point calculation and the Markov chain nature of the problem, the probability to 6 figures is 330.721. (The script is a naive implementation without consideration for efficiency. It still runs quickly.)

```

1 library(expm)
2 N <- 30

```

```

3
4 surroundNeighbors <- function(site) {
5   belowSite <- if (site[1] == N) NULL else c(site
6     [1]+1, site[2])
7   leftSite <- if (site[2] == 1) NULL else c(site
8     [1], site[2]-1)
9   aboveSite <- if (site[1] == 1) NULL else c(site
10    [1]-1, site[2])
11   rightSite <- if (site[2] == N) NULL else c(site
12    [1], site[2]+1)
13   neighbors <- rbind(belowSite, leftSite,
14     aboveSite, rightSite)
15 }
16
17 site2i <- function(site) {
18   site[1] + (site[2] - 1) * N
19 }
20
21 i2site <- function(i) {
22   c( ( (i-1) %% N + 1 ), ((i-1) %/% N + 1) )
23 }
24
25 T = matrix(0, N^2, N^2)
26
27 for (i in 1:N^2) {
28   nbrs <- surroundNeighbors( i2site(i) )
29   for (k in 1:nrow(nbrs)) {
30     nbr <- nbrs[k, ]
31     T[i, site2i(nbr)] <- 1/nrow(nbrs)
32   }
33 }
34
35 complementT50 <- 1 - T %>% 50
36 emptyCells <- sum(apply(complementT50, 2, prod))
37 emptyCells
38

```

The following Julia scripts are efficient implementations of the simulation and theoretical analyses.

```

1 const N = 30
2
3 neighbors(c::Tuple{Int, Int}) =
4   filter!([c .+ d for d in ((1, 0), (-1, 0), (0, 1)
5     , (0, -1))]) do new_c
6     all(x -> 1 <= x <= N, new_c)
7   end
8

```

```

7  # The key element of this function is removing new
   # potential locations that
8  # are out of bounds.
9
10 const NEI = [neighbors((i, j)) for i in 1:N, j in 1:N
   ]
11
12 function sim(steps)
13     fleas = [(i, j) for i in 1:N, j in 1:N]
14     for _ in 1:steps
15         for i in eachindex(fleas)
16             fleas[i] = rand(NEI[fleas[i]...])
17             # note the splatting, expanding to
multiple positional args
18         end
19     end
20     unoccupied = trues(N, N)
21     for c in fleas
22         unoccupied[c...] = false
23     end
24     return sum(unoccupied)
25 end
26 # The idea of the simulation is to initialize it with
   # 900 fleas, each
27 # starting on a different square. Then each of them
   # moves randomly to one of
28 # the locations it is allowed to occupy. Finally,
   # count the number of
29 # unoccupied squares.
30
31 using Statistics
32 using Random
33 Random.seed!(1234);
34
35 simres = [sim(50) for _ in 1:10_000]
36 mean(simres)
37 # Additionally compute the 90% confidence interval
   # for the estimator using bootstrapping:
38 quantile([mean(rand(simres, length(simres))) for _ in
   1:10_000],
39          [0.05, 0.95])

```

```

1  const N = 30
2
3  neighbors(c::Tuple{Int, Int}) =

```

```

4      filter!([c .+ d for d in ((1, 0), (-1, 0), (0, 1)
5      , (0, -1))]) do new_c
6          all(x -> 1 <= x <= N, new_c)
7      end
8  # The key element of this function is removing new
9  # potential locations that
10 # are out of bounds.
11
12 const NEI = [neighbors((i, j)) for i in 1:30, j in 1:
13 N]
14
15 # build a transition
16 # probability matrix for the problem. For this, first
17 # create two helper
18 # functions that recode (i, j) position of a flea to
19 # its numeric index:
20 c2i(c::Tuple{Int, Int}) = c[1] + (c[2] - 1) * N
21 i2c(i::Int) = reverse(divrem(i - 1, N)) .+ (1, 1)
22
23 # The location TRANS[i, j] encodes the probability
24 # that flea starting from
25 # location i (encoded using linear index) ends up in
26 # location j. Therefore
27 # the sum of probabilities in rows are all equal to
28 # one.
29 const TRANS = zeros(N^2, N^2)
30 for i in 1:N^2
31     ni = c2i.(neighbors(i2c(i)))
32     TRANS[i, ni] .= 1 / length(ni)
33 end
34
35 # the TRANS ^ 50 matrix encodes probability that flea
36 # starting from
37 # location i ends up in location j after 50 moves. 1
38 # .- TRANS ^ 50 is
39 # a matrix, where TRANS[i, j] is the probability that
40 # flea
41 # starting in position i is not in position j after
42 # 50 moves. Since
43 # fleas move independently prod(1 .- TRANS^50, dims
44 # =1) gives a
45 # probability for each cell that it is not occupied
46 # by any flea. Using
47 # linearity of expectation again, the expected number
48 # of
49 # unoccupied cells is sum(prod(1 .- TRANS^50, dims=1)
50 # ).

```

```

35 |
36 | round(sum(prod(1 .- TRANS^50, dims=1)), digits=6)

```

**Remark .27.** This problem is slightly adapted from the Project Euler Problem 213. The solution and the Julia scripts are adapted from Flea circus for the New Year celebration. A detailed discussion of the simulation approach is at How should one approach Project Euler problem 213?. Another solution using multinomial distributions is at R-bloggers: Flea Circus

1: The algebra is tedious but routine. Checking just the first entry is representative. The first-row, first-column entry of  $P_{X|X}$  is

$$\frac{p_1^2}{(p_1 + p_3)(p_1 + p_2)} + \frac{p_3^2}{(p_1 + p_3)(p_3 + p_4)}$$

and the second-row, first-column entry of  $P_{X|X}$  is

$$\frac{p_1 p_2}{(p_2 + p_4)(p_3 + p_4)} + \frac{p_3 p_4}{(p_2 + p_4)(p_3 + p_4)}.$$

The dot product of the row-vector  $f = (p_1 + p_3, p_2 + p_4)$  with the elements making this column gives

$$\frac{p_1^2}{(p_1 + p_2)} + \frac{p_3^2}{(p_3 + p_4)} + \frac{p_1 p_2}{(p_1 + p_2)} + \frac{p_3 p_4}{(p_3 + p_4)}.$$

The sum of the first and third fractions simplifies to  $p_1$ , the sum of the second and fourth fractions simplifies to  $p_3$  and the total is  $p_1 + p_3$ .

2:

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x, y) \, dy &= \int_{-\infty}^{\infty} \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)}} \, dy \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{\rho^2 x^2 - 2\rho xy + y^2}{2(1-\rho^2)}} \, dy \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{(\rho x - y)^2}{2(1-\rho^2)}} \, dy \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{z^2}{2(1-\rho^2)}} \, dz \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \int_{-\infty}^{\infty} e^{-\frac{u^2}{2}} \sqrt{1-\rho^2} \, du \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2}{2(1-\rho^2)}} e^{\frac{\rho^2 x^2}{2(1-\rho^2)}} \sqrt{2\pi(1-\rho^2)} \\
&= \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}.
\end{aligned}$$

3:

$$\begin{aligned}
f_{x|y}(x|y) &= f(x, y)/f_y(y) \\
&= \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)}} / \frac{1}{\sqrt{2\pi}} e^{-y^2/2} \\
&= \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)} + \frac{(1-\rho^2)y^2}{2(1-\rho^2)}} \\
&= \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{x^2-2\rho xy+\rho^2 y^2}{2(1-\rho^2)}} \\
&= \frac{1}{\sqrt{2\pi(1-\rho^2)}} e^{-\frac{(x-\rho y)^2}{2(1-\rho^2)}}.
\end{aligned}$$

1:

$$\begin{aligned}
\int_0^\infty \frac{e^{-\theta} \theta^x}{x!} e^{-\theta} d\theta &= \frac{1}{x!} \int_0^\infty e^{-2\theta} \theta^x d\theta \\
&= \frac{1}{x!} \cdot \frac{1}{2^{x+1}} \int_0^\infty e^{-2\theta} (2\theta)^x d(2\theta) \\
&= \frac{1}{x!} \cdot \frac{1}{2^{x+1}} \cdot x!
\end{aligned}$$

where the last equality is the factorial property of the Gamma integral.

2:

$$\begin{aligned}
\int_0^\infty \frac{2^{x+1} \theta^{x+x'} e^{-3\theta}}{x!x'!} d\theta &= \frac{2^{x+1}}{x!x'!} \int_0^\infty \theta^{x+x'} e^{-3\theta} d\theta \\
&= \frac{2^{x+1}}{3^{x+x'+1} x!x'!} \int_0^\infty (3\theta)^{x+x'} e^{-3\theta} d(3\theta) = \frac{2^{x+1}}{3^{x+x'+1} x!x'!} (x+x')! \\
&= \frac{2^{x+1}}{3^{x+x'+1}} \binom{x+x'}{x}.
\end{aligned}$$

3:

$$\begin{aligned}
&\left(\frac{1}{1+\alpha}\right)^a \sum_{x=0}^\infty \frac{(a)_x}{x!} \left(\frac{\alpha}{\alpha+1}\right)^x \\
&= \left(\frac{1}{1+\alpha}\right)^a \left[1 + \frac{a}{1!} \left(\frac{\alpha}{\alpha+1}\right) + \frac{a(a+1)}{2!} \left(\frac{\alpha}{\alpha+1}\right)^2 + \dots\right] \\
&= \left(\frac{1}{1+\alpha}\right)^a \left[1 - \frac{-a}{1!} \left(\frac{\alpha}{\alpha+1}\right) + \frac{-a(-a-1)}{2!} \left(\frac{\alpha}{\alpha+1}\right)^2 + \dots\right] \\
&= \left(\frac{1}{1+\alpha}\right)^a \left[1 - \frac{\alpha}{\alpha+1}\right]^{-a} = 1
\end{aligned}$$

where the next-to-last equality is from the general Binomial Expansion or equivalently the Taylor expansion of  $(1+z)^{-a}$ .



4: Move terms in the denominator not depending on  $\lambda$  out of the integral and combine like terms in the numerator.

$$\begin{aligned} k(x, y) &= \int_0^\infty \frac{e^{-\lambda(\alpha+1)/\alpha} \lambda^{a+x-1}}{\Gamma(a+x)(\alpha/(\alpha+1))^{a+x}} \cdot \frac{e^{-\lambda} \lambda^y}{y!} d\lambda \\ &= \frac{1}{\Gamma(a+x)(\alpha/(\alpha+1))^{a+x} y!} \int_0^\infty e^{-\lambda((\alpha+1)/\alpha+1)} \lambda^{a+x+y-1} d\lambda. \end{aligned}$$

Let  $z = \frac{2\alpha+1}{\alpha} \lambda$ , so  $d\lambda = \frac{\alpha}{2\alpha+1} dz$ . Then the integral becomes

$$\begin{aligned} \int_0^\infty e^{-\lambda((\alpha+1)/\alpha+1)} \lambda^{a+x+y-1} d\lambda &= \int_0^\infty e^{-z} z^{a+x+y-1} \left( \frac{\alpha}{2\alpha+1} \right)^{a+x+y} dz \\ &= \Gamma(a+x+y) \left( \frac{\alpha}{2\alpha+1} \right)^{a+x+y}. \end{aligned}$$

5: Use the definition of the Meixner polynomial

$$M_j(x; a, \alpha) = {}_2F_1(-j, -x; a; -\alpha)$$

in terms of the Gauss series for the regular hypergeometric function with  $a = -j$ ,  $b = -x$ ,  $c = a$  and  $z = -\alpha$ . For negative integer values of  $a$  the Gauss series terminates as a degree  $j$  polynomial. Then directly  $M_0(x) = 1$ , and  $M_1(x) = 1 + \frac{(-1)(-x)(-\alpha)}{1! \cdot a} = 1 - \frac{\alpha}{a}x$  and  $M_2(x) = 1 + \frac{(-1)(-x)(-\alpha)}{1! \cdot a} + \frac{(-2)(-1)(-x)(-x+1)\alpha^2}{2! \cdot a(a+1)} = 1 - \frac{\alpha(\alpha+a+1)}{a(a+1)}x + \frac{\alpha^2}{a(a+1)}x^2$ .

6: For  $j = k = 0$ ,

$$\sum_{x=0}^{\infty} M_0(x) M_0(x) m(x) = \sum_{x=0}^{\infty} m(x) = 1$$

because  $m(x)$ , the negative binomial distribution, is a probability distribution. This matches the given

$$\frac{(1+\alpha)^0 0!}{(a)_0} \delta_{00} = 1.$$

For  $j = 0$  and  $k = 1$

$$\begin{aligned} \sum_{x=0}^{\infty} M_0(x) M_1(x) m(x) &= \sum_{x=0}^{\infty} M_1(x) m(x) = \sum_{x=0}^{\infty} \left( 1 - \frac{\alpha}{a}x \right) m(x) \\ &= \sum_{x=0}^{\infty} m(x) - \frac{\alpha}{a} \sum_{x=0}^{\infty} x m(x) = 1 - \frac{\alpha}{a} \cdot a \cdot \frac{\alpha}{\alpha+1} \cdot \frac{1}{1/\alpha+1} = 1 - \frac{\alpha^2}{(\alpha+1)^2} \end{aligned}$$

by using the mean of the negative binomial distribution.

For  $j = k = 1$

$$\begin{aligned}
 & \sum_{x=0}^{\infty} M_1(x) M_1(x) m(x) \\
 &= \sum_{x=0}^{\infty} \left(1 - \frac{\alpha}{a} x\right)^2 m(x) \\
 &= \sum_{x=0}^{\infty} m(x) - 2 \frac{\alpha}{a} \sum_{x=0}^{\infty} x m(x) + \frac{\alpha^2}{a^2} \sum_{x=0}^{\infty} x^2 m(x) \\
 &= 1 - 2 \frac{\alpha}{a} \cdot a \cdot \frac{\alpha}{\alpha+1} \cdot \frac{1}{1/\alpha+1} + \frac{\alpha^2}{a^2} a \cdot \frac{\alpha}{\alpha+1} \cdot \frac{1}{(1/\alpha+1)^2} = 1 - 2\alpha^2 + \frac{\alpha^3(\alpha+1)}{\alpha}
 \end{aligned}$$

by using the mean and variance of the negative binomial distribution.

7: Follow [Chi78, pages 4 and 176].

The generating function definition of the Meixner polynomials  $m_n(x, \beta, c)$  is

$$\left(1 - \frac{w}{c}\right)^x (1-w)^{-x-\beta} = \sum_{\nu=0}^{\infty} m_{\nu}(x; \beta, c) \frac{w^{\nu}}{n!}$$

The binomial expansion for the first factor in  $G(x, w)$  is  $\left(1 - \frac{w}{c}\right)^x$  is

$$\left(1 - \frac{w}{c}\right)^x = \sum_{\nu=0}^{\infty} (-1)^{\nu} \binom{x}{\nu} \frac{w^{\nu}}{c^{\nu}} = \sum_{\nu=0}^{\infty} \frac{(x)_n}{k!} \frac{w^{\nu}}{c^{\nu}}$$

where  $(x)_n$  is the falling Pochhammer symbol or falling factorial  $x(x-1)(x-2) \cdots (x-(n-1))$ .

The binomial expansion for the second factor in  $G(x, w)$  is

$$(1-w)^{-x-\beta} = \sum_{\nu=0}^{\infty} (-1)^{\nu} \binom{-x-\beta}{\nu} w^{\nu}.$$

Then multiplying the two expansions, collecting terms in powers of  $w$  gives for the coefficient  $n$

$$m_n(x, \beta, c) = (-1)^n n! \sum_{\nu=0}^n \binom{x}{\nu} \binom{-x-\beta}{n-\nu} c^{-\nu}.$$

The factor  $n!$  results from “multiply in  $n!$  and divide out  $n!$ ” to introduce the  $n!$  in denominator of the definition which was not originally present in the binomial expansions. The  $(-1)^n$  results from the  $(-1)^{\nu}$  from the first factor binomial expansion and the  $(-1)^{n-\nu}$  from the second factor binomial expansion. The  $c^{-\nu}$  comes from the denominator in the expansion of the first term.

Since  $\binom{x}{\nu} = \frac{1}{\nu!} x(x-1) \cdots (x-\nu+1)$  has degree  $\nu$  and  $\binom{-x-\beta}{n-\nu} = \frac{1}{(n-\nu)!} (-x-\beta)(-x-\beta-1) \cdots (-x-\beta-(n-\nu-1))$  has degree  $n-\nu$ ,  $m_n(x, \beta, c)$  is a polynomial of degree  $n$ .

Now an identity in the parameters of the Meixner polynomials

$$\begin{aligned}
 m_n(-x - \beta; \beta, c_{-1}) &= (-1)^n n! \sum_{\nu=0}^n \binom{-x - \beta}{\nu} \binom{-(x - \beta) - \beta}{n - \nu} (c^{-1})^{-\nu} \\
 &= (-1)^n n! \sum_{\nu=0}^n \binom{-x - \beta}{\nu} \binom{x}{n - \nu} c^\nu \\
 &= c^n (-1)^n n! \sum_{\nu=0}^n \binom{-x - \beta}{\nu} \binom{x}{n - \nu} c^{\nu - n} \\
 &= c^n (-1)^n n! \sum_{\nu_1=0}^n \binom{-x - \beta}{n - \nu_1} \binom{x}{\nu_1} c^{\nu_1} \\
 &= c^n m_n(x; \beta, c).
 \end{aligned}$$

- 1: Consider a representative node  $j$  with  $1 \leq j \leq n - 1$  with load  $q_j$  and neighboring node with load  $q_{j+1}$ . After one Markov chain step by  $P_{1/2}$  of load exchange the expected gain would be  $\frac{1}{2}q_{j+1} - \frac{1}{2}q_j$ . If  $q_{j+1} > q_j$ , the gain is positive, one-half of the load imbalance shifts from  $j + 1$  to  $j$ . If  $q_{j+1} < q_j$ , the gain is negative, one-half of the load imbalance shifts from  $j$  to  $j + 1$ . For the end node  $n$ , the calculation is similar.
- 2: The matrix  $(\mathbf{1}\mathbf{1}^T)$  has 1 in every entry. The matrix-vector product  $(\mathbf{1}\mathbf{1}^T) \mathbf{1}$  sums the rows, giving  $n\mathbf{1}$ , then  $(1/n) (\mathbf{1}\mathbf{1}^T) \mathbf{1} = \mathbf{1}$ .
- 3: There are two urns I and II containing a total of  $n$  balls. The state of the Markov chain is the number of balls in urn I so the number of states is  $n + 1$ . At each turn, with probability  $p$  a ball is taken from urn II and moved to urn I or with complementary probability  $q$  a ball is moved from urn I to urn II. If there are no balls in urn I then with probability  $q$  urn I stays empty. Similarly for the last state if urn I has all  $n$  balls.
- 4: Use the sum-to-product identity for cosines:

$$\cos(\theta) + \cos(\phi) = 2 \cos\left(\frac{\theta + \phi}{2}\right) \cdot \cos\left(\frac{\theta - \phi}{2}\right)$$

to directly get

$$\begin{aligned}
 &\frac{1}{2} \left( \cos\left(\frac{(2j-1)\pi}{n}\right) + \cos\left(\frac{(2j+1)\pi}{n}\right) \right) \\
 &= \cos\left(\frac{1}{2} \left[ \frac{(2j-1)\pi}{n} + \frac{(2j+1)\pi}{n} \right]\right) \cos\left(\frac{1}{2} \left[ \frac{(2j-1)\pi}{n} - \frac{(2j+1)\pi}{n} \right]\right) \\
 &= \cos\left(\frac{\pi}{n}\right) \cos\left(\frac{2j\pi}{n}\right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \frac{1}{n} \left[ \cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{2j\pi}{n}\right) \right] \\
 &= \frac{2}{n} \cos\left(\frac{1}{2} \left[ \frac{2j\pi}{n} + \frac{\pi}{n} \right]\right) \cos\left(\frac{1}{2} \left[ \frac{2j\pi}{n} - \frac{\pi}{n} \right]\right) \\
 &= \frac{2}{n} \cos\left(\frac{(2j-1)\pi}{2n}\right) \cos\left(\frac{(2j+1)\pi}{2n}\right).
 \end{aligned}$$

5: Directly computing, the characteristic polynomial is  $p(x) = \frac{1}{2}x(x-1)(2x^2 - 1)$ . The eigenvalues are  $1, \sqrt{2}/2, 0 - \sqrt{2}/2$  corresponding to  $\cos(0 \cdot \pi/4), \cos(1 \cdot \pi/4), \cos(2 \cdot \pi/4), \cos(3 \cdot \pi/4)$  respectively.

6: Consider the  $n \times n$  tridiagonal matrix

$$\begin{pmatrix} q & p & 0 & \cdots & 0 \\ q & 0 & p & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & q & 0 & p \\ 0 & \cdots & 0 & q & p \end{pmatrix}.$$

The equations connecting the eigenvalue  $\lambda$  and the components  $u_i$  of the eigenvectors are

$$(\lambda) \quad \lambda u_1 = qu_1 + pu_2$$

$$(\lambda) \quad \lambda u_2 = qu_1 + pu_3$$

$$(\lambda) \quad \vdots \quad \vdots$$

$$(\lambda) \quad \lambda u_{n-1} = qu_{n-2} + pu_n$$

$$(\lambda) \quad \lambda u_n = qu_{n-1} + pu_n.$$

Equations (.5) through (.7) are satisfied by  $u_j = s^j$  provided

$$\begin{aligned}
 \lambda s^2 &= qs + ps^3 \\
 \vdots \quad \vdots \\
 \lambda s^{n-1} &= qs^{n-2} + ps^n.
 \end{aligned}$$

These are all equivalent to  $\lambda s = q + ps^2$ , or  $ps^2 - \lambda s + q = 0$ , so the solutions are  $s_+ = \frac{\lambda + \sqrt{\lambda^2 - 4pq}}{2p}$  and  $s_- = \frac{\lambda - \sqrt{\lambda^2 - 4pq}}{2p}$ . Then

the solution is of the form

$$\begin{aligned} u_1 &= A(\text{lambd}\mathbf{a})s_+ + B(\text{lambd}\mathbf{a})s_- \\ u_2 &= A(\text{lambd}\mathbf{a})s_+^2 + B(\text{lambd}\mathbf{a})s_-^2 \\ &\vdots \\ u_{n-1} &= A(\text{lambd}\mathbf{a})s_+^{n-1} + B(\text{lambd}\mathbf{a})s_-^{n-1} \\ u_n &= A(\text{lambd}\mathbf{a})s_+^n + B(\text{lambd}\mathbf{a})s_-^n. \end{aligned}$$

Apply equation (.4) to get

$$\begin{aligned} \text{lambd}\mathbf{a}(As_+ + Bs_-) &= q(As_+ + Bs_-) + p(As_+^2 + Bs_-^2) \\ 0 &= A[(\text{lambd}\mathbf{a} - q)s_+ - ps_+^2] + B[(\text{lambd}\mathbf{a} - q)s_- - ps_-^2] \\ (.9) \quad 0 &= A[q(s_+ - 1)] + B[q(s_- - 1)]. \end{aligned}$$

Applying the last equation (.8) to get

$$\begin{aligned} \text{lambd}\mathbf{a}(As_+^n + Bs_-^n) &= q(As_+^{n-1} + Bs_-^{n-1}) + p(As_+^n + Bs_-^n) \\ 0 &= As_+^{n-1}[(\text{lambd}\mathbf{a}s_+ - q) - ps_+] + Bs_-^{n-1}[(\text{lambd}\mathbf{a}s_- - q) - ps_-] \\ 0 &= As_+^{n-1}[ps_+^2 - ps_+] + Bs_-^{n-1}[ps_-^2 - ps_-] \\ (.10) \quad 0 &= As_+^n p[s_+ - 1] + Bs_-^n p[s_- - 1] \\ (.11) \quad -As_+^n p[s_+ - 1] &= Bs_-^n p[s_- - 1]. \end{aligned}$$

Substituting equation (.9) get

$$s_+^n = s_-^n.$$

Note that  $s_+s_- = q/p$  so  $s_+^{2n} = (q/p)^n$  and  $s_-^{2n} = (q/p)^n$ . That is, both  $s_+$  and  $s_-$  are  $(2n)$ th roots of  $(q/p)^n$ . Therefore,  $s_+$  and  $s_-$  can be written in the form

$$e^{i\pi j/n} = \sqrt{q/p} \left( \cos\left(\frac{\pi j}{n}\right) + i \sin\left(\frac{\pi j}{n}\right) \right)$$

for  $j = 0, 1, 2, \dots, 2n - 1$ .

Thus, the eigenvalues  $\text{lambd}\mathbf{a}$  are among the solutions of

$$s_+(\text{lambd}\mathbf{a}) = \sqrt{q/p} e^{i\pi j/n}$$

or

$$\begin{aligned}
 \frac{\lambda + \sqrt{\lambda^2 - 4pq}}{2p} &= \sqrt{\frac{q}{p}} e^{i\pi j/n} \\
 \lambda + \sqrt{\lambda^2 - 4pq} &= \sqrt{4pq} e^{i\pi j/n} \\
 \sqrt{\lambda^2 - 4pq} &= -\lambda + e^{i\pi j/n} \\
 \lambda^2 - 4pq &= \lambda^2 - 2\lambda \sqrt{4pq} e^{i\pi j/n} + 4pq e^{2i\pi j/n} \\
 -4pq &= -2\lambda \sqrt{4pq} e^{i\pi j/n} + 4pq e^{2i\pi j/n} \\
 \frac{4pq}{2\sqrt{4pq} e^{i\pi j/n}} + \frac{4pq e^{i\pi j/n}}{2\sqrt{4pq}} &= \lambda \\
 \sqrt{4pq} \left( \frac{e^{-i\pi j/n}}{2} + \frac{e^{i\pi j/n}}{2} \right) &= \lambda \\
 \sqrt{4pq} \cos \pi j/n &= \lambda.
 \end{aligned}$$

So to each  $j$  there is a root  $\lambda_j$ , namely

$$\lambda_j = \sqrt{4pq} \cos(\pi j/n) \quad j = 0, 1, 2, \dots, 2n-1.$$

However, some of these roots are repeated, since

$$\cos(\pi j/n) = \cos(\pi(2n-j)/n)$$

for  $j = 1, \dots, n$ . So there are  $n$  eigenvalues  $\lambda_1 = 1$  and  $\lambda_j = \sqrt{4pq} \cos\left(\frac{(j-1)\pi}{n}\right)$  for  $j = 2, \dots, n$ . This is maximized for  $p = q = 1/2$ .

7: A simple R program using only base functions:

```

1 r <- 0
2 p <- 1/2
3 q <- 1 - p
4
5 for (n in 2:8) {
6
7   P <- diag(r, n, n)
8   P[ row(P) - col(P) == 1] <- p
9   P[ row(P) - col(P) == -1] <- q
10  P[1, 1] = q
11  P[n, n] = p
12
13  cat("Size of matrix: ", n, "Eigenvalues: ",
14      unlist(eigen( P, only.values=TRUE )), "\n")
15 }

```

1: Here the  $X$  process and the  $Y$  process definitely have different starting distributions. But the  $X$  process and the  $Y$  process both have the same (simple)

transition probabilities. To be explicit, suppose  $Y_0 = 0$ , and the first 5 transitions for  $Y$  are  $0 \rightarrow 1$ ,  $1 \rightarrow 1$ ,  $1 \rightarrow 1$ ,  $1 \rightarrow 0$ , and  $0 \rightarrow 1$ . Then the states are  $Y_0 = 0$ ,  $Y_1 = 1$ ,  $Y_2 = 1$ ,  $Y_3 = 1$ ,  $Y_4 = 0$ ,  $Y_5 = 1$ . By the definition of  $X_t$ ,  $X_0 = 0$ ,  $X_1 = Y_0 = 0$ ,  $X_2 = Y_1 = 1$ ,  $X_3 = Y_2 = 1$ ,  $X_4 = Y_3 = 1$ ,  $X_5 = Y_4 = 0$ . Then, for example

$$\mathbb{P}[X_{t+1} = 0 \mid X_t = 0] = \mathbb{P}[Y_t = 0 \mid Y_{t-1} = 0] = 1/2$$

and likewise for the other three transition probabilities. Thus,  $X_t$  also has transition probability matrix  $P$ . Furthermore, this same construction shows that  $(X_t, Y_t)$  is a Markov process on the 4-element state space. However

$$\mathbb{P}[X_1 = 0 \mid X_0 = 0, Y_0 = 0] = 1 \neq 1/2.$$

Essentially, the joint process is correct, but the marginals are not correct.

2: