Discrete Time Markov Chain (DTMC)

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Sources

- Taylor & Karlin, *An Introduction to Stochastic Modeling*, 3rd edition. Chapters 3-4.
- Ross, *Introduction to Probability Models*, 8th edition, Chapter 4.

1 Overview: stochastic process

A. A *stochastic process* is a collection of random variables $\{X_t, t \in T\}$.

B. A *sample path* or *realization* of a stochastic process is the collection of values assumed by the random variables in one realization of the random process, e.g., the sample path $x_1, x_2, x_3, ...$, when $X_1 = x1, X_2 = x_2, X_3 = x_3, ...$ We may speak of the probability of a realization, and we mean $P(X_1 = x1, X_2 = x_2, X_3 = x_3, ...)$, for example.

C. The *state space* is the collection of all possible values the random variables can take on, i.e., it is the *sample space* of the random variables. For example, if $X_i \in [0, \infty)$ represent random times for all i, then the *state space* of the stochastic process is $[0, \infty)$.

D. Often, the index set T is associated with time, sometimes even when it does not actually represent time. In this description, the stochastic process has a *state* that evolves in time. For example, the process may start in state $X_1 = 3$, then evolve to state $X_2 = 4$, and much later enters the state $X_{100} = 340$. The index set may also be associated with space, for example $T = \mathbb{R}^2$ for the real plane.

E. Classifying stochastic processes.

Stochastic processes can be classified by whether the *index set* and *state space* are discrete or continuous.

		State Space	
		discrete	continuous
Index	discrete	discrete time Markov chain (dtmc)	not covered
Set	continuous	continuous time Markov chain (ctmc)	diffusion process

1. Random variables of a discrete time process are commonly written X_n, where $n = 0, 1, 2, ...$
2. Random variables of a continuous time process are commonly written $X(t)$, where $t \in T$, and T is often, though certainly not always $[0, \infty)$.

F. Short history of stochastic processes illustrating close connection with physical processes.

1. 1852: dtmc invented to model rainfall patterns in Brussels
2. 1845: branching process (type of dtmc) invented to predict the chance that a family name goes extinct.
3. 1905: Einstein describes Brownian motion mathematically
4. 1910: Poisson process describes radioactive decay
5. 1914: birth/death process (type of ctmc) used to model epidemics

G. Relationship to other mathematics

1. mean behavior of the ctmc is described by ordinary differential equations (ODEs)
2. diffusion processes satisfy stochastic differential equations (SDEs), from stochastic calculus

2 Introduction to Discrete Time Markov Chain (DTMC)

A. **Definition:** A discrete time stochastic process $\{X_n, n = 0, 1, 2, ...\}$ with discrete state space is a Markov chain if it satisfies the **Markov property**.

$$P(X_n = i_n | X_0 = i_0, X_1 = i_1, ..., X_{n-1} = i_{n-1}) = P(X_n = i_n | X_{n-1} = i_{n-1}) \tag{1}$$

where i_k for all $k = 0, 1, ..., n$ are realized states of the stochastic process.

B. **Brief history**

1. Markov chain named after Andrei Markov, a Russian mathematician who invented them and published first results in 1906.
2. Andrey Kolmogorov, another Russian mathematician, generalized Markov's results to countably infinite state spaces.
3. Markov Chain Monte Carlo technique is invented by Metropolis, Rosenbluth, Rosenbluth, Teller and Teller in 1953 in statistical physics. Allows simulation/sampling from complicated distributions/models.

C. **Definition: one-step transition probabilities** $p_{ij}^{n,n+1}$

The one-step transition probability is the probability that the process, when in state i at time n, will next transition to state j at time $n+1$. We write

$$p_{ij}^{n,n+1} = P(X_{n+1} = j | X_n = i) \tag{2}$$

1. $0 \leq p_{ij}^{n,n+1} \leq 1$ since the transition probabilities are (conditional) probabilities.
2. $\sum_{j=0}^{\infty} p_{ij}^{n,n+1} = 1$ since the chain must transition somewhere and summing over all j is an application of the addition law for a set of disjoint and exhaustive events.

D. **Definition: time homogeneity**

When the one-step transition probabilities do not depend on time, so that

$$p_{ij}^{n,n+1} = p_{ij} \tag{3}$$

for all n, then the one-step transition probabilities are said to be *stationary* and the Markov chain is also said to be stationary or *time homogeneous*.

E. **Definition: one-step transition matrix or transition matrix or Markov matrix** The *one-step transition matrix*, P , is formed by arranging the one-step transition probabilities into a matrix:

$$P = \begin{pmatrix} p_{00} & p_{01} & p_{02} & \cdots \\ p_{10} & p_{11} & p_{12} & \cdots \\ p_{20} & p_{21} & p_{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{4}$$

1. P is a square matrix, possibly of infinite dimension if the state space is countable.
2. The rows sum to 1, by properties of one-step transition probabilities given above.

F. **Examples**

1. **A simple weather forecasting model**

   Let X_i be an indicator random variable that indicates whether it will rain on day i. The index set is $T = \{0, 1, 2, ...\}$ It is discrete and truly represents time. The *state space* is $\{0, 1\}$. It is clearly discrete.

   Assume that whether it rains tomorrow depends only on whether it is raining (or not) today, and no previous weather conditions (Markov property).

   Let α be the probability that it will rain tomorrow, given that it is raining today. Let β be the probability that it will rain tomorrow, given that it is *not* raining today.

   The Markov matrix is

   $$P = \begin{pmatrix} \alpha & 1-\alpha \\ \beta & 1-\beta \end{pmatrix} \tag{5}$$

2. **A slightly more complex weather forecasting model**

   Suppose that you believe that whether it rains tomorrow is actually influences not only by whether it is raining today, but also by whether it was raining yesterday. At first glance, it seems that you cannot use a Markov chain model for this situation, since the future depends on the present as well as the past. Fortunately, by redefining the state space, and hence the future, present, and past, one can still formulate a Markov chain.

   Define the state space as the rain state of pairs of days. Hence, the possible states are $(0, 0)$, indicating that it rained today and yesterday, $(0, 1)$, indicating that it rained yesterday and did not rain today, $(1,0)$, and $(1,1)$, defined similarly.

In this *higher order* Markov chain, certain transitions are immediately for- bidden, for one cannot be allowed to change the state of a day when making a transition. So, for example, $(0,0)$ cannot transition to $(1,0)$. As we move forward in time, today will become yesterday, and the preceding transition suggests that what was rain today became no rain when viewed from tomorrow. The only transitions with non-zero probability are shown below, where the order of states along the rows and columns of the matrix are $(0,0),(0,1),(1,0),(1,1)$.

$$P = \begin{pmatrix} 0.7 & 0.3 & 0 & 0 \\ 0 & 0 & 0.4 & 0.6 \\ 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0.2 & 0.8 \end{pmatrix} \tag{6}$$

Note in the preceding, the probability of rain after two days of rain is 0.7. The probability of rain after one day of rain followed by one day of no rain is 0.4. The probability of rain after only one day of rain is 0.5. Finally, the probability of rain after two days of no rain is 0.2.

3. **The random walk**

   A Markov chain whose state space is $i = 0, \pm 1, \pm 2, ...$ is a random walk if for some $0 < p < 1$, where

$$p_{i,i+1} = p = 1 - p_{i,i-1} \tag{7}$$

   One useful application is to gambling models.

4. **DNA models**

   Analogous DNA models can be formulated. Here the state space for the simple, first-order model is $\{0,1,2,3\}$, where 0 may represent A, 1 may represent C, 2 may represent G, and 3 may represent T. The state space for the slightly more complex, second-order model is $\{00,01,02,03,10,11,...\}$, which has 4^2 possible states. Higher order models are also possible, with a corresponding increase in the number of states. While it might not seem intuitive why such a model could possibly describe a DNA sequence (think human genome for instance), a little thought can suggest why it might work better than an even simpler model. Suppose I ask you to predict for me the 10th nucleotide in a sequence I have just obtained for a gene in the human genome. You can come up with some kind of prediction based on what you know about nucleotide content of the human genome, but if I also told you the 9th nucleotide of the sequence, you may be able to make a better prediction based on your knowledge not only about the nucleotide content of the human genome, but knowledge about behavior of segments of the sequences (codons), for example. Indeed, it is not hard to show that a first order Markov chain often fits DNA sequence data better than a Independent and identically distributed random variables model.

5. **Automobile insurance**

   Suppose auto insurance costs are determined by the a positive integer value indicating the risk of the policyholder, plus the car and coverage level.

   Each year, the policyholder's state is updated according to the number of claims made during the year.

   Let $s_i(k)$ be the state of a policyholder who was in state i and made k claims last year. These are fixed numbers determined by the insurance company. Randomness enters via the number of claims made by a policyholder.

   Suppose the number of claims made by a policy holder is a Poisson random variable with parameter λ. Then, the transition probabilities are

$$p_{i,j} = \sum_{k:s_i(k)=j} e^{-\lambda} \frac{\lambda^k}{k!} \tag{8}$$

   Consider the following hypothetical table of $s_i(k)$:

		Next state if			
State	Annual Premium	0 claims	1 claims	2 claims	≥ 3 claims
1	200	1	2	3	4
2	250	1	3	4	4
3	400	2	4	4	4
4	600	3	4	4	4

Suppose $\lambda = 1$. Using the above table we can compute the transition probability matrix

$$P = \begin{pmatrix} 0.37 & 0.37 & 0.18 & 0.08 \\ 0.37 & 0 & 0.37 & 0.26 \\ 0 & 0.37 & 0 & 0.63 \\ 0 & 0 & 0.37 & 0.63 \end{pmatrix} \tag{9}$$

3 Chapman-Kolmogorov Equations

A. **Definition: n-step transition probabilities**

$$p_{ij}^n = P(X_{n+k} = j | X_k = i) \tag{10}$$

for $n \geq 0$ and states i, j.

By analogy to the 1-step case, we can define n-step transition probability matrices $P^{(n)} = (p_{ij}^n)$.

B. **Result: Chapman-Kolmogorov equations**

$$p_{ij}^{n+m} = \sum_{k=0}^{\infty} p_{ik}^n p_{kj}^m \tag{11}$$

for all $n, m \geq 0$ and for all states i, j.

Proof:

$$
\begin{aligned}
p_{ij}^{n+m} &= P(X_{n+m} = j | X_0 = i) \\
&= \sum_{k=0}^{\infty} P(X_{n+m} = j, X_n = k | X_0 = i) P(X_n = k | X_0 = i) \\
&= \sum_{k=0}^{\infty} P(X_{n+m} = j | X_n = k, X_0 = i) \\
&= \sum_{k=0}^{\infty} p_{kj}^{m} p_{ik}^{n} \qquad (12)
\end{aligned}
$$

C. **Additional Results:**

1. Another compact way to write Chapman-Kolmogorov equations:

$$p^{(n+m)} = P^{(n)} P^{(m)} \qquad (13)$$

2. By induction,

$$P^{(n)} = P^{n} \qquad (14)$$

D. **Examples**

1. **Simple Forecasting Model**

Suppose $\alpha = 0.7$ and $\beta = 0.4$, so

$$P = \begin{pmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{pmatrix} \qquad (15)$$

What is the probability that it will still be clear in 4 days, given that it is clear today? We need P^4.

$$P^2 = P \cdot P = \begin{pmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{pmatrix} \qquad (16)$$

and

$$P^4 = P^2 \cdot P^2 = \begin{pmatrix} 0.5749 & 0.4251 \\ 0.5668 & 0.4332 \end{pmatrix} \qquad (17)$$

The entry we seek is $p_{11}^4 = 0.5749$, so there is approximately a 57% chance that it will be clear in 4 days.

2. **More Complex Forecasting Model**

   Now, compute the probability that it will rain on Saturday given that it rained today Thursday and didn?t rain yesterday Wednesday.

$$P^{(2)} = P^2 = \begin{pmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{pmatrix} \times \begin{pmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{pmatrix}$$
$$= \begin{pmatrix} 0.49 & 0.12 & 0.21 & 0.18 \\ 0.35 & 0.20 & 0.15 & 0.30 \\ 0.20 & 0.12 & 0.20 & 0.48 \\ 0.10 & 0.16 & 0.10 & 0.64 \end{pmatrix} \tag{18}$$

4 Unconditional probabilities

In order to compute unconditional probabilities, like "What is the probability it will rain on Tuesday?", we'll need to define the initial state distribution. A Markov chain is fully specified once the transition probability matrix and the initial state distribution have been defined.

A. **Definition: initial state distribution**

   The initial state distribution is a probability distribution defined over the first state of the chain X_0.

$$P(X_0 = i) = \alpha_i \tag{19}$$

   for all $i = 0, 1, ...$

B. Now we can compute unconditional probabilities.

   1. Computing probability of state j at particular time n:

$$P(X_n = j) = \sum_{i=0}^{\infty} P(X_n = j | X_0 = i) P(X_0 = i) = \sum_{i=0}^{\infty} p_{ij}^n \alpha_i \tag{20}$$

2. Computing probability of a chain realization:

$$\begin{aligned}
&P(X_0 = i_0, X_1 = i_1, ..., X_n = i_n) \\
&= P(X_0 = i_0)P(X_1 = i_1|X_0 = i_0)P(X_2 = i_2|X_0 = i_0, X_1 = i_1) \\
&\quad \cdots P(X_n|X_0 = i_0, X_{n-1} = i_{n-1})
\end{aligned} \tag{21}$$

The Markov property allows us to simplify

$$\begin{aligned}
&P(X_0 = i_0, X_1 = i_1, ..., X_n = i_n) \\
&= P(X_0 = i_0)P(X_1 = i_1|X_0 = i_0)P(X_2 = i_2|X_1 = i_1) \\
&\quad \cdots P(X_n|X_{n-1} = i_{n-1})
\end{aligned} \tag{22}$$

and finally we obtain

$$P(X_0 = i_0, X_1 = i_1, ..., X_n = i_n) = \alpha_{i_0} p_{i_0 i_1} p_{i_1 i_2} \cdots p_{i_{n-1} i_n} \tag{23}$$

C. **Example.** Using the simple weather forecasting model, what is the probability that it will rain on Monday given that there was a 90% chance or rain today?

$$P(X_4 = 1) = \alpha_0 p_{01}^4 + \alpha_1 p_{11}^4 = 0.10 \times 0.4251 + 0.90 \times 0.4332 = 0.43239 \tag{24}$$

5 Irreducible chains

A. Introduction: classification of states

Note, define the 0-step transition probabilities as follows

$$p_{ij}^0 = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \tag{25}$$

1. **Definition:** State j is said to be *accessible* from state i if $p_{ij}^n > 0$ for some $n \geq 0$.
2. **Definition:** Two states i and j are said to *communicate* if they are accessible to each other, and we write $i \leftrightarrow j$.
   a. The relation of communication is an equivalence relation, i.e.,
      - **Reflexive:** $i \leftrightarrow i$ because $p_{ii}^0 = 1$.

- **Communicative:** If $i \leftrightarrow j$ then $j \leftrightarrow i$
- **Transitive:** If $i \leftrightarrow j$ and $j \leftrightarrow k$, then $i \leftrightarrow k$.

b. This equivalence relation divides the state space of a Markov chain into non-overlapping classes.

3. **Definition:** A *class property* is a property of the state that if true of one member in a class, is true of all members in that class.

B. **Definition:** A Markov chain is *irreducible* if there is only one equivalence class of states, i.e., all states communicate with each other.

C. **Examples:**

1. The Markov chain with transition probability matrix

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{3} & \frac{2}{3} \end{pmatrix} \tag{26}$$

is irreducible.

2. The Markov chain with transition probability matrix

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{27}$$

has three classes $\{0, 1\}$ and $\{2\}$ and $\{3\}$ and is not irreducible.

D. 1. **Definition:** A transition probability matrix P is *regular* if there exists an n, such that P^n has strictly positive entries, i.e., $p_{ij}^n > 0$ for all $i, j \geq 0$.

2. **Claim:** a Markov chain with a regular transition probability matrix is irreducible.

Note that for the n where $P^n > 0$, $p_{ij}^n > 0$ for all $i, j \geq 0$, hence all states i in the state space communicate with all other states j.

3. **Method:** One way to check for irreducible Markov chains is to roughly calculate $P^2, P^4, P^8, ...$ to see if eventually all entries are

strictly positive. Consider, the 3×3 matrix from the first example above.

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

First, encode entries as + or 0 and call this encoded matrix Q.

$$Q = \begin{pmatrix} + & + & 0 \\ + & + & + \\ 0 & + & + \end{pmatrix} \tag{28}$$

Then,

$$Q^2 = \begin{pmatrix} + & + & + \\ + & + & + \\ + & + & + \end{pmatrix} \tag{29}$$

Therefore, the Markov matrix P is irreducible.

6 Recurrence and transience

Let f_i be the probability that starting in state i, the process reenters state i at some later time $n > 0$. Note, this concept is related but different from the concept of *accessibility*. In the example below, $0 \leftrightarrow 1$, but the chain is not guaranteed to return to 0 if it starts there,so $f_0 < 1$.

$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{30}$$

A. Definitions related to recurrence and transience.

1. **Definition:** If $f_i = 1$, then the state i is said to be *recurrent*.
2. **Definition:** We define the random variable R_i to be the first return time to recurrent state i

$$R_i = \min_{n \geq 1} \{X_n = i | X_0 = i\} \tag{31}$$

3. **Definition:** A recurrent state is *positive recurrent* if it recurs with finite mean time, i.e., $E[R_i] < \infty$.

4. **Definition:** In contrast, a recurrent state is *null recurrent* if it recurs only after an infinite mean wait time, i.e., $E[R_i] = \infty$.

   Note: Null recurrent states can only occur in infinite state Markov chains, for example the symmetric random walks in one and two dimensions are null recurrent.

5. **Definition:** State i is said to be an *absorbing state* if $p_{ii} = 1$. An absorbing state is a special kind of positive recurrent state.

   Absorption is the process by which Markov chains absorb when absorbing states are present.

6. **Definition:** If $f_i < 1$, then the state i is a *transient* state.

B. Claims and results related to recurrence and transience.

1. **Claim:** A recurrent state will be visited infinitely often.

   Suppose the recurrent state i is visited only $T < \infty$ times. Since T is the last visit, there will be no more visits to state i after time T. This is a contradiction since the probability that i is visited again after time T is $f_i = 1$.

2. **Claim:** The random number of times a transient state will be visited is finite and distributed as a geometric random variable.

   Consider a chain that starts in state i. Then, with probability $1 - f_i \geq 0$, the chain will never re-enter state i again. The probability that the chain visits state i n more times is

   $$P(n \text{ visits}) = f_i^n(1 - f_i) \tag{32}$$

   where we recognize the pmf[1] of a Geometric distribution. The expectation of the Geometric distribution is finite.

3. **Theorem:** State i is recurrent if $\sum_{n=1}^{\infty} p_{ii}^n = \infty$ and transient if $\sum_{n=1}^{\infty} p_{ii}^n < \infty$.

   Proof:

[1]a probability mass function (pmf) is a function that gives the probability that a discrete random variable is exactly equal to some value.

Let

$$I_n = \begin{cases} 1 & \text{if } X_n = i \\ 0 & \text{if } X_n \neq i \end{cases} \tag{33}$$

indicate whether the chain is in state i at the nth time point. Then

$$\sum_{n=1}^{\infty} I_n$$

is the total number of visits to state i after chain initiation. Take the expectation,

$$\begin{aligned} E\left[\sum_{n=1}^{\infty} I_n\right] &= \sum_{n=1}^{\infty} E(I_n | X_0 = i) \\ &= \sum_{n=1}^{\infty} P(X_n = i | X_0 = i) \\ &= \sum_{n=1}^{\infty} p_{ii}^n \end{aligned} \tag{34}$$

4. **Corollary:** If state i is recurrent and j communicates with i, then j is recurrent.

   Proof:

   Because i and j communicate, there exist m and n such that

   $$p_{ij}^m > 0 \quad , \quad p_{ji}^n > 0 \tag{35}$$

   By Chapman-Kolmogorov,

   $$p_{jj}^{m+k+n} \geq p_{ji}^n p_{ii}^k p_{ij}^m \tag{36}$$

   Sum over all possible k

   $$\sum_{k=1}^{\infty} p_{jj}^{m+k+n} \geq p_{ji}^n p_{ij}^m \sum_{k=1}^{\infty} p_{ii}^k = \infty \tag{37}$$

5. **Claim:** Recurrence (positive and null) and transience are class properties. This result is an obvious consequence of the above Corollary.

6. **Claim:** All states in a finite-state, irreducible Markov chain are recurrent. Because some states in a finite-state Markov chain must be recurrent, in fact *all* are recurrent since there is only one equivalence class in an irreducible Markov chain and recurrence is a class property.
7. **Claim:** Not all states can be transient in a finite-state Markov chain. Suppose there are N states in the state space of a finite-state Markov chain. Let N_i be the finite number of visits to state $0 \le i \le N-1$. Then after $\sum_{i=1}^{N-1} N_i$ steps in time, the chain will not be able to visit any state $i = 0, ..., N-1$, a contradiction.

C. **Examples:**

1. Determine the transient states in the following Markov matrix.
$$\begin{pmatrix} 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0.35 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{38}$$
Verify that all states communicate, therefore, all states must be recurrent and the chain is irreducible.
2. Determine the transient, recurrent, and absorbing states in the following Markov matrix.
$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & & & & & \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & & & & & \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & & & & & \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{4} & \frac{1}{4} & 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{39}$$
This chain consists of three classes $\{0,1\}$, $\{2,3\}$, and $\{4\}$. The first two classes are recurrent. The last is transient.
3. Suppose the transition probability matrix were modified as
$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{40}$$
Then, there are four classes $\{0\}$, $\{1\}$, $\{2,3\}$, and $\{4\}$ and the first two are recurrent absorbing states.

7 Periodicity of Markov chain

A. **Definition:** The *period* of state i is the greatest common divisor of all n such that $p_{ii}^n > 0$. In other words, if we consider all the times at which we could possibly be in state i, then the period is the greatest common divisor of all those times.

   If the state i can be revisited at any time, then the period is 1.

   If the state i can be revisited every two time points, then the period is 2.

   If the state i can never be revisited (i.e., diagonal entry in that ith row is 0), the the period is *defined* as 0.

B. **Definition:** A Markov chain is *aperiodic* if every state has period 0 or 1.

C. **Example:**

   Confirm the period of the following chain is 3.

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{41}$$

8 Ergodicity

A. **Definition:** A state is ergodic if it is positive recurrent and aperiodic.

B. **Claim:** Ergodicity is a class property.

C. **Definition:** A Markov chain is *ergodic* if its states are aperiodic and positive recurrent.

9 Example

Random walk on the integers with transition probabilities:

$$p_{i,i+1} = p = 1 - p_{i,i-1} \tag{42}$$

All states communicate with each other, therefore all states are either recurrent or transient. Which is it?

Focus on state 0 and consider $\sum_{n=1}^{\infty} p_{00}^n$. Clearly,

$$p_{00}^{2n} = 0 \quad , \quad n = 1, 2, ... \tag{43}$$

because we cannot return to 0 with an uneven number of steps.

Furthermore, we can only return to 0 in $2n$ steps if we take n steps away and n steps toward, so

$$p_{00}^{2n} = \binom{2n}{n} p^n (1-p)^n \tag{44}$$

Employing the Stirling approximation

$$n! \sim n^{n+1/2} e^{-n} \sqrt{2\pi} \tag{45}$$

where $a_n \sim b_n$ if $\lim_{n\to\infty} \frac{a_n}{b_n} = 1$. Therefore,

$$p_{00}^{2n} \sim \frac{[4p(1-p)]^n}{\sqrt{\pi n}} \tag{46}$$

By definition of $\sim$, it is not hard to see that $\sum_{n=1}^{\infty} p_{00}^n$ will only converge if

$$\sum_{n=1}^{\infty} \frac{[4p(1-p)]^n}{\sqrt{\pi n}} < \infty \tag{47}$$

But $4p(1-p) < 1$ except when $p = \frac{1}{2}$. Thus, if $p = \frac{1}{2}$, then $\sum_{n=1}^{\infty} p_{00}^n = \infty$ and the chain is recurrent, otherwise $\sum_{n=1}^{\infty} p_{00}^n < \infty$ and the chain is transient.

One may also show that the *symmetric random walk* in two dimensions is recurrent. However, all random walks in more than 2 dimensions are transient.

10 First-Step Analysis

A. Preliminaries

We discuss first-step analysis for finite-state discrete time Markov chains $\{X_n, n \geq 0\}$. Label the finite states $0, 1, 2, ..., N-1$. There a total of N states.

Generically, the technique of first-step analysis can be used to solve many complex questions regarding *time homogeneous* Markov chains. It solves the problem by breaking the process into what happens in the first step and what happens in all the remaining steps. Because stationary Markov chains are memoryless (the future is independent of the past) and probabilistically constant in time, the future of the chain after the first step is probabilistically identical to the future of the chain before the first step. The result is a set of algebraic equations for the unknowns we seek.

First-step analysis, in its simplest form, answers questions about absorption into absorbing states. Therefore, suppose $S = \{S_0, S_1, ..., S_{N-r-1}\}, r \leq N$ are all the absorbing states in a Markov chain. Based on our understanding of recurrence and transience, it is clear that the chain must ultimately end up in one of the absorbing states in S. There are details we may wish to know about this absorption event.

1. **Definition:** The *time to absorption* T_i is the time it takes to enter some absorbing state in S given the chain starts in state i.

$$T_i = \min_{n \geq 0} \{X_n \geq r | X_0 = i\} \tag{48}$$

2. **Definition:** The hitting probability for state $S_i \in S$ is the probability that a Markov chain enters state S_i before entering any other state in S.

$$U_{ik} = P(X_{T_i} = k | X_0 = i) \tag{49}$$

In addition, remember our trick for answering the question "What is the probability that the Markov chain enters a state or group of states before time n?" Often, while the original Markov chain may not have any absorbing states (i.e., $S = \emptyset$), questions about the Markov chain can be reformulated as questions about absorption into particular states or groups of states. In this case, one constructs a novel Markov chain where certain states are converted into absorbing states.

B. Technique: Finding the probability that a Markov Chain has entered (and perhaps left) a particular set of states $\mathscr{A}$ by time n.

1. Construct a new Markov chain with modified state space transition probabilities

$$q_{ij} = \begin{cases} 1 & \text{if } i \in \mathscr{A}, j = i \\ 0 & \text{if } i \in \mathscr{A}, j \neq i \\ p_{ij} & \text{otherwise} \end{cases} \tag{50}$$

The new Markov chain has transition probability matrix $Q - (q_{ij})$ and be- haves just like the original Markov chain until the state of the chain enters set $\mathscr{A}$. Therefore, both chains will have the same behavior with respect to the question.

2. **Example.** Suppose a person receives 2 (thousand) dollars each month. The amount of money he spends during the month is $i = 1, 2, 3, 4$ with probability P_i and is independent of the amount he has. If the person has more than 3 at the end of a month, he gives the excess to charity. Suppose he starts with 5 after receiving his monthly payment (i.e. he was in state 3 right before the first month started). What is the probability that he has 1 or fewer within the first 4 months? We will show that as soon as $X_j \leq 1$, the man is at risk of going into debt, but if $X_j > 1$ he cannot go into debt in the next month.

Let $X_j \leq 3$ be the amount the man has at the end of month j.

The original Markov chain matrix is infinite, which makes the analysis a little tricky.

$$P = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & & \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \cdots & 0 & P_4 & P_3 & P_2 & P_1 & 0 \\ & \cdots & 0 & P_4 & P_3 & P_2 & P_1 \\ & & \cdots & 0 & P_4 & P_3 & P_2 + P_1 \end{pmatrix} \tag{51}$$

To answer the question, we would define the modified Markov chain

$$Q' = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & 0 & 1 & 0 & 0 & 0 \\ \cdots & 0 & 0 & 1 & 0 & 0 \\ \cdots & 0 & P_4 & P_3 & P_2 & P_1 \\ \cdots & 0 & 0 & P_4 & P_3 & P_2 + P_1 \end{pmatrix} \tag{52}$$

but we can't work with an infinite matrix. To proceed, we note that if we start with $X_j > 1$, then we can only enter condition $X_j \le 1$ by entering state 0 or 1. For example, the worst state > 1 the man can be in the previous month is 2. He then earns 2 and spends, at most, 4 with probability P_4, to end up, at worst, with 0. In short, we claim that states $\{....,-2,-1\}$ are inaccessible in the modified Markov chain, so we can ignore them to get a finite and workable matrix

$$Q = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ P_4 & P_3 & P_2 & P_1 \\ 0 & P_4 & P_3 & P_2 + P_1 \end{pmatrix} \tag{53}$$

Suppose $P_i = \frac{1}{4}$ for all $i = 1,2,3,4$. We compute Q^4 for the first four months

$$Q^4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{93}{256} & \frac{129}{256} & \frac{13}{256} & \frac{21}{256} \\ \frac{36}{256} & \frac{165}{256} & \frac{21}{256} & \frac{34}{256} \end{pmatrix} \tag{54}$$

The man started in state 3. The probability he ends in state ≤ 1 by the 4th month is $\frac{36}{256} + \frac{165}{256} = \frac{201}{256} \approx 0.79$, where we sum the probability that he first goes to state ≤ 1 via 0 $(\frac{36}{256})$ or via 1 $(\frac{165}{256})$.

C. Standard form of Markov matrix.

Assume that of the N states $0,1,...,r-1$ are transient and states $r,...,N-1$ are absorbing. If the states are currently not in this order, one can re-order and re-number them, so that they are.

With this ordering of the states, the Markov matrix is in the standard form, which can be written as

$$P = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix} \tag{55}$$

where we have split P into 4 submatrices: Q is an $r \times r$ matrix, R is an $r \times N - r$ matrix, 0 is an $N - r \times r$ matrix filled with 0's and I is an $N - r \times N - r$ identity matrix. An identity matrix is a matrix with 1's along the diagonal and 0's elsewhere, for example the 2×2 identity matrix is

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

D. Time Until Absorption.

(System-of-equations solution)

1. Sub-Questions: many similar questions exist that can be answered in the same mathematical framework.
   a. How long (many steps) before absorption (to any absorbing states)?
   b. If you win \$5 every time transient state k is visited, how much money do you expect to win before the game is over (absorption)?
2. Preliminaries
   a. Let $g(j)$ be a random function that maps each state to some value.

      Let

      $$w_i = E\left[\sum_{n=0}^{T_i - 1} g(X_n) | X_0 = i\right] \tag{56}$$

      be the expected value of the sum of $g(j)$ over all transient states prior to absorption. To facilitate later derivation, we define $g(l) = 0$ for all absorbing states $l \geq r$.
   b. Let $g(l) = 1$ for all transient states l. Then w_i is the expected time until absorption given the chain starts in state i.
   c. Let $g(l) = \delta_{lk}$ which is 1 for transient state k and otherwise 0. Then w_i is the expected number of visits to state k before absorption. Later we call this W_{ik}.

d. Let $g(l)$ be the dollar amount you win or lose for each state of the chain. Then w_i is the expected amount of your earnings until absorption of the chain.

3. Derivation

$$
\begin{aligned}
w_i &= E\left[\sum_{n=0}^{T-1} g(X_n)|X_0 = i\right] \qquad \text{(by definition)} \\
&= E\left[\sum_{n=0}^{\infty} g(X_n)|X_0 = i\right] \quad , \quad (g(X_n) = 0 \text{ for } n \geq T) \\
&= E\left[g(X_0) + \sum_{n=1}^{\infty} g(X_n)|C_0 = i\right] \\
&= g(i) + \sum_{n=1}^{\infty} E[g(X_n)|X_0 = i] \quad , \quad \text{(expectation of sums)} \\
&= g(i) + \sum_{n=1}^{\infty}\sum_{j=0}^{N-1} g(j)P(X_n = j|X_0 = i) \quad \text{(definition of expectation)} \\
&= g(i) + \sum_{n=1}^{\infty}\sum_{j=0}^{N-1}\sum_{l=0}^{N-1} g(j)P(X_n = j|X_0 = i, X_1 = l)p_{il} \\
&= g(i) + \sum_{n=1}^{\infty}\sum_{j=0}^{N-1}\sum_{l=0}^{N-1} g(j)P(X_n = j|X_1 = l)p_{il} \ \text{ Markov property} \\
&= g(i) + \sum_{l=0}^{N-1} p_{il}\sum_{n=1}^{\infty}\sum_{j=0}^{N-1} g(j)P(X_n = j|X_1 = l) \ \text{ rearrange sums}
\end{aligned}
\tag{57}
$$

Re-index the remaining portion of the Markov chain $\{X_1, X_2, ...\}$ to start from 0 to make the next step more obvious. For example, define $Y_{i-1} = X_i$ for all $i = 1, 2, ...$ After that, we back out of the sums, reversing the arguments above.

$$
\begin{aligned}
w_i &= g(i) + \sum_{l=0}^{N-1} p_{il} \sum_{m=0}^{\infty} \sum_{j=0}^{N-1} g(j) P(Y_m = j | Y_0 = l) \\
&= g(i) + \sum_{l=0}^{N-1} p_{il} \sum_{m=0}^{\infty} E[g(Y_m) | Y_0 = l] \\
&= g(i) + \sum_{l=0}^{N-1} p_{il} E\left[\sum_{m=0}^{\infty} g(Y_m) | Y_0 = l\right] \\
&= g(i) + \sum_{l=0}^{N-1} p_{il} E\left[\sum_{m=0}^{T-1} g(Y_m) | Y_0 = l\right] \\
&= g(i) + \sum_{l=0}^{N-1} p_{il} w_{il} \qquad (58)
\end{aligned}
$$

(Matrix solution)

1. Preliminaries. **Expected "time" before absorption:** We use w_i to denote the expectation of random variables defined on the time and transient states visited before absorption.

$$w_i = E\left[\sum_{n=0}^{T_i-1} g(X_n) | X_0 = i\right] \qquad (59)$$

Let W_{ik} be the expected number of visits to the transient state k before absorption given that the chain started in state i. In other words, W_{ik} is a special case of w_i when

$$g(l) = \delta_{lk} \qquad (60)$$

We can arrange the W_{ik} into an $r \times r$ matrix called W.

Similarly, let W_{ik}^n be the expected number of visits to the transient state k through time n (which may or may not precede absorption), given that the chain started in state i. In other words, W_{ik}^n is given by an equation similar to that of w_i, namely

$$W_{ik}^n = E\left[\sum_{m=0}^{n} g(X_m) | X_0 = i\right] \qquad (61)$$

We can arrange the W_{ik}^n into an $r \times r$ matrix called W^n.

Please note that as $n \to \infty$, n will eventually be certain to exceed absorption time T_i. Since we defined $g(l) = 0$ for all absorbing states $l \geq r$, then $W^n \to W$ as $n \to \infty$. We will use this fact later.

2. **Lemma.** $W = (I - Q)^{-1}$ where Q is the submatrix in the standard Markov chain defined above and W is constructed from elements W_{ik} as described above.

   Proof:

   One can perform a derivation similar to the one above to obtain equations for W_{ik}^n

$$W_{ik}^n = \delta_{ik} + \sum_{j=0}^{r-1} p_{ij} W_{jk}^{n-1} \tag{62}$$

   In matrix form, this equation is

$$W^n = I + QW^{n-1} \tag{63}$$

   where I is an identity matrix.

   Let $n \to \infty$. On both sides of this equation, $W^n, W^{n-1} \to W$, so we obtain

$$W = I + QW \tag{64}$$

   which we can solve to find W.

$$\begin{aligned}
W &= I + QW \\
W - QW &= I \\
IW - QW &= I \quad \text{(multiplication by identity)} \\
(I - Q)W &= I \quad \text{(distributive rule)} \\
IW &= (I - Q)^{-1} I \quad \text{(definition of inverse)} \\
W &= (I - Q)^{-1} \quad \text{(multiplication by identity)}
\end{aligned} \tag{65}$$

E. Hitting Probabilities.

(System-of-equations solution)

1. **Derivation:**

Consider what can happen in the first step and what happens to the target after the first step has been taken. The table is simply

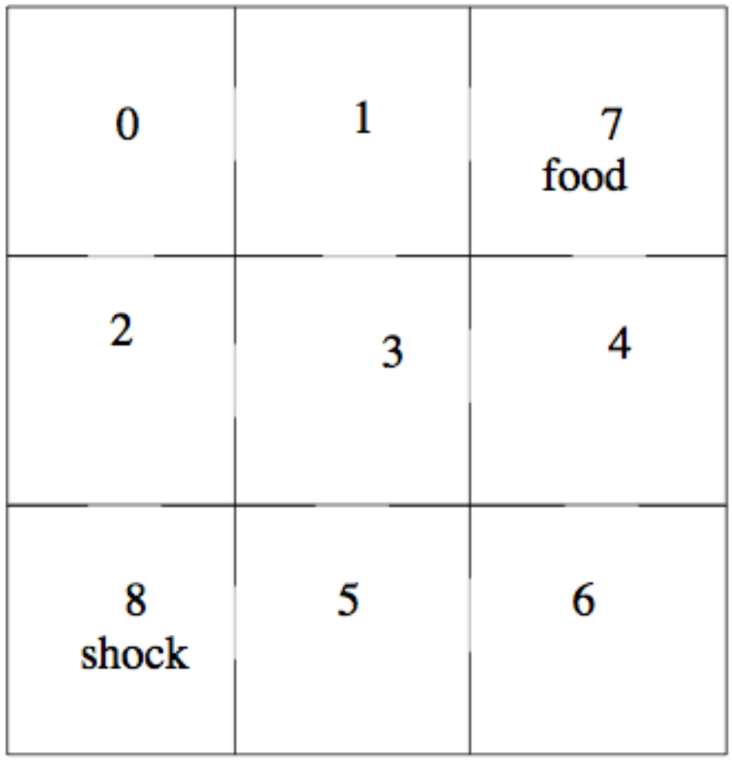
Possible first step (j)	Probability	What's the target from here?
$j = k$	p_{ik}	$P(X_{T_i} = k \mid X_0 = i, X_1 = k) = 1$
$j \neq k, j = r, ..., N-1$	p_{ij}	$P(X_{T_i} = k \mid X_0 = i, X_1 = j) = 0$
$j - 1, ..., r$	p_{ij}	$P(X_{T_i} = k \mid X_0 = i, X_1 = j) = U_{jk}$

an application of the law of total probability, where we consider all possible outcomes of the first step. Repeating the above table in mathematical equations, we have

$$
\begin{aligned}
U_{ik} &= \sum_{n=0}^{N-1} P(X_{T_i} = k, X_1 = j \mid X_0 = i) \quad i = 0, ..., r-1 \\
&= \sum_{n=0}^{N-1} P(X_{T_i} = k \mid X_0 = i, X_1 = j) P(X_1 = j \mid X_0 = i) \\
&= \sum_{n=0}^{N-1} P(X_{T_i} = k \mid X_1 = j) p_{ij} \\
&= p_{ik} + 0 + \sum_{j=0}^{r-1} p_{ij} U_{jk} \qquad (66)
\end{aligned}
$$

The key ingredient is to recognize that $P(X_{T_i} = k \mid X_1 = j) = P(X_{T_i} = k \mid X_0 = j)$ because of the Markov property and time homogeneity.

2. **Example:** Rat in a Maze



The matrix is

$$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{67}$$

We seek equations for U_{i7}, the probability that the mouse will eat food in compartment 7 before being shocked in compartment 8 given that it starts in compartment i.

$$
\begin{aligned}
U_{07} &= \tfrac{1}{2}U_{17} + \tfrac{1}{2}U_{27} \\
U_{17} &= \tfrac{1}{3}U_{07} + \tfrac{1}{3}U_{37} + \tfrac{1}{3} \\
U_{27} &= \tfrac{1}{3}U_{07} + \tfrac{1}{3}U_{37} + \tfrac{1}{3} \times 0 \\
U_{37} &= \tfrac{1}{4}U_{17} + \tfrac{1}{4}U_{27} + \tfrac{1}{4}U_{47} + \tfrac{1}{4}U_{47} \\
U_{47} &= \tfrac{1}{3} + \tfrac{1}{3}U_{37} + \tfrac{1}{3}U_{67} \\
U_{57} &= \tfrac{1}{3}U_{37} + \tfrac{1}{3}U_{67} + \tfrac{1}{3} \times 0 \\
U_{67} &= \tfrac{1}{2}U_{47} + \tfrac{1}{2}U_{57} \\
U_{77} &= 1 \\
U_{87} &= 0
\end{aligned}
\tag{68}
$$

3. **Example:** Return to 0 in a random walk.

We are interested in determining the probability that the drunkard will ever return to 0 given that he starts there when $p > \frac{1}{2}$. While there are no absorbing states in this chain, we can introduce one in order to answer the question. Let 0 become an absorbing state as soon as the drunkard takes his first step. Then, we are interested in the hitting probability of state 0.

Consider the first step. He moves to 1 or -1. First we deal with -1, by showing that he *must* return to 0 from -1.

Define the random variable

$$
Y_i = \begin{cases} 1 & \text{with probability } p \\ -1 & \text{with probability } 1-p \end{cases} \tag{69}
$$

which has mean $E[Y_n] = 2p - 1$. When $p > \frac{1}{2}$, then $E[Y_n] > 0$. The Strong Law of Large Numbers implies

$$
\frac{\sum_{i=1}^{n} Y_i}{n} \to 2p - 1 > 0
$$

Thus, $X_n = \sum_{i=1}^{n} Y_i > 0$, which implies if $X_i = -1$, the chain must eventually return through 0 to the positive numbers.

Now assume the first move was to 1. What is the probability of return to 0. Well, condition on all possible second steps gives

$$U_{10} = pU_{20} + (1-p)U_{00} = pU_{10}^2 + 1 - p \tag{70}$$

which is a quadratic equation with roots

$$U_{10} = 1 \quad \text{or} \quad U_{10} = \frac{1-p}{p} \tag{71}$$

Thus, the unconditional probability of hitting 0 is

$$p\frac{1-p}{p} + 1 - p = 2(1-p) \tag{72}$$

Similarly, when $p < \frac{1}{2}$, we have $U_{00}^* = 2p$ and in general

$$U_{00}^* = 2\min(p, 1-p) \tag{73}$$

(Matrix solution)

1. **Lemma:** $U = WR$

   Proof:

   $$P^2 = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix} \times \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix} = \begin{pmatrix} Q^2 & R + QR \\ 0 & I \end{pmatrix} \tag{74}$$

   and, in general,

   $$P^n = \begin{pmatrix} Q^n & (I + Q + Q^2 + \cdots + Q^{n-1})R \\ 0 & I \end{pmatrix} \tag{75}$$

   Now we consider $n \to \infty$.

   The following paragraph is a rough argument for completeness, but not necessary for the proof. The matrix Q^n consists of n-step transition probabilities p_{ij}^n where i and j are transient states. The chain will ultimately absorb into one of the absorbing states, so as n gets large, the probability of transitioning to a transient state after n steps goes to 0 and $Q^n \to 0$.

   It is the upper right quadrant that interests us most. There we find a matrix series. Suppose there is a matrix V^n which equals the nth series, i.e.,

$$V^n = 1 + Q + Q^2 + \cdots + Q^n \tag{76}$$

Then we have

$$V^n = 1+Q+Q^2+\cdots+Q^n = I+Q(1+Q+Q^2+\cdots+Q^{n-1} = I+QV^{n-1} \tag{77}$$

This equation looks familiar. In fact, we argued that W^n satisfies such an equation, and therefore we conclude that $V^n = W^n$ and in the limit, the upper right quadrant goes to WR.

All together

$$P^\infty = \begin{pmatrix} 0 & WR \\ 0 & I \end{pmatrix} \tag{78}$$

After absorption time T, the chain is in an absorbing state and there is no further change in the state, thus

$$U_{ik} = P(X_T = k|X_0 = i) = P(X_\infty = k|X_0 = i) = P_{ij}^\infty = (WR)_{ik} \tag{79}$$

Thus,

$$U = WR \tag{80}$$

11 Limiting Distribution

Consider the Markov matrix

$$P = \begin{pmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{pmatrix} \tag{81}$$

and examine the powers of the Markov matrix

$$P^2 = \begin{pmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{pmatrix}$$

$$P^4 = \begin{pmatrix} 0.5749 & 0.4281 \\ 0.5668 & 0.4332 \end{pmatrix}$$

$$P^8 = \begin{pmatrix} 0.572 & 0.428 \\ 0.570 & 0.430 \end{pmatrix}$$

One should observe that the matrix rows become more and more similar.

For example, both $p_{00}^{(8)}$ and $p_{10}^{(8)}$ are very similar. As time progresses (here, by the 00 10 time we have taken 8 time steps), the probability of moving into state 0 is virtually independent of the starting state (here, either 0 or 1).

Indeed, it turns out that under certain conditions the n-step transition probabilities

$$p_{ij}^{n} \to \pi_j \tag{82}$$

approach a number, we'll call π_j, that is independent of the starting state i.

Another way to say this is that for n sufficiently large, the probabilistic behavior of the chain becomes independent of the starting state, i.e.,

$$P(X_n = j | X_0 = i) = P(X_n = j) \tag{83}$$

A.
1. **Theorem:** For irreducible, *ergodic* Markov chain, the limit $\lim_{n \to nifty} p_{ij}^{n}$ exists and is independent of i. Let

$$\pi_j = \lim_{n \to nifty} p_{ij}^{n} \tag{84}$$

   for all $j \geq o$. In addition, the π_j are the unique, nonnegative solution of

$$\pi_j = \sum_{i=0} \pi_i p_{ij} \quad , \quad \sum_{j=0}^{\infty} \pi_j = 1 \tag{85}$$

   Proof is given in Karlin and Taylor's *A First Course in Stochastic Processes.*

2. Matrix equation for $\pi = (\pi_0, \pi_1, \pi_2, ...)$ is $\pi = \pi P$.
3. Pseudo-proof:

   Suppose that the limit mentioned in the above theorem exists for all j. By the law of total probability, we have

$$\begin{aligned} P(X_{n+1} = j) &= \sum_{i=0}^{\infty} P(X_{n+1} = j | X_n = i) P(X_n = i) \\ &= \sum_{i=0}^{\infty} p_{ij} P(X_n = i) \end{aligned}$$

Let $n \to \infty$ on both sides. If one can bring the limit inside the sum, then

$$\pi_j = \sum_{i=0} \pi_i p_{ij}$$

which is the equation claimed in the theorem.

B. Stationary Distribution.

1. **Definition:** stationary distribution

   If there exist π_j that satisfy $\pi_j = \sum_j p_{ij}\pi_i$ and $\sum_i \pi_i = 1$, the π_j is called a *stationary distribution*. However, be clear that if $\lim_{n\to\infty} p_{ij}^n \neq \pi_j$, then it is *not* a *limiting distribution*. Some points:

   a. The *limiting distribution* **does not exist** for periodic chains.

   b. A *limiting distribution* is a *stationary distribution*.

   c. Neither the *limiting distribution* nor the *stationary distribution* need exist for irreducible, null recurrent chains.

2. Fundamental result.

   Lemma: If the irreducible, positive recurrent chain is started with initial state distribution equal to the *stationary distribution*, then $P(X_n = j) = \pi_j$ for all future times n.

   Proof: (by induction)

   Show true for $n = 1$.

   $$P(x_1 = j) = \sum_i p_{ij}\pi_i = \pi_j \qquad \text{(by limiting distribution equation).}$$

   Assume it is true for $n-1$, so $P(X_{n-1} = j) = \pi_j$,

   Show true for n.

$$\begin{aligned} P(X_n = j) &= \sum_i P(X_n = j | X_{N-1} = i) P(X_{n-1} = i) \\ &= \sum_i p_{ij}\pi_i \quad , \quad \text{(by induction hypothesis).} \\ &= \pi_j \qquad \text{(by limiting distribution equation).} \end{aligned} \tag{86}$$

C. Long-Run Proportion.

Claim: π_j is the long-run proportion of time the process spends in state j.

Proof (for aperiodic chains):

Recall that if a sequence of numbers $a_0, a_1, a_2, ...$ converges to a, then the sequence of partial averages

$$s_m = \frac{1}{m}\sum_{j=0}^{m-1} a_j$$

also converges to a.

Consider the partial sums

$$\frac{1}{m}\sum_{k=0}^{m-1} p_{ij}^k$$

In the limit, as $m \to \infty$, these partial sums converge to π_j. But recall

$$\begin{aligned}
&= \sum_{k=0}^{m-1} E[1\{X_k = j\}|X_0 = i] \\
&= E\left[\sum_{k=0}^{m-1} 1\{X_k = j\}|X_0 = i\right] \\
&= E[\#\text{ time steps spent in state } j]
\end{aligned}$$

Here, we have used $1\{X_k = j\}$ is the indicator function that is 1 when $X_k = j$ and 0 otherwise. Therefore, the partial sums created above converge to the proportion of time the chain spends in state j.

D. Examples.

1. Weather.

   Recall the simple Markov chain for weather (R = rainy, S = sunny) with transition matrix

$$P = \begin{array}{c} \\ R \\ S \end{array} \begin{array}{c} \begin{array}{cc} R & S \end{array} \\ \left\| \begin{array}{cc} \alpha & 1-\alpha \\ \beta & 1-\beta \end{array} \right\| \end{array} \tag{87}$$

To find the limiting distribution, we must solve the following equations

$$\begin{aligned}\pi_R &= \pi_R p_{RR} + \pi_S p_{SR} = \alpha \pi_R + \beta \pi_S \\ \pi_S &= \pi_R p_{RS} + \pi_S p_{SS} = (1-\alpha)\pi_R + (1-\beta)\pi_S\end{aligned} \tag{88}$$

with solution

$$\pi_R = \frac{\beta}{1+\beta-\alpha} \quad , \quad \pi_R = \frac{1-\alpha}{1+\beta-\alpha} \tag{89}$$

2. Two-Day Weather Model.

$$P = \begin{array}{c} \\ 0 = (R,R) \\ 1 = (R,S) \\ 2 = (S,R) \\ 3 = (S,S) \end{array} \begin{array}{c} \begin{array}{cccc} 0 = (R,R) & 1 = (R,S) & 2 = (S,R) & 3 = (S,S) \end{array} \\ \left\| \begin{array}{cccc} \alpha & 1-\alpha & 0 & 0 \\ 0 & 0 & \beta & 1-\beta \\ \alpha & 1-\alpha & 0 & 0 \\ 0 & 0 & \beta & 1-\beta \end{array} \right\| \end{array} \tag{90}$$

To find the limiting distribution, we must solve the following equations

$$\begin{aligned}\pi_0\alpha + \pi_2\alpha &= \pi_0 \\ \pi_0(1-\alpha) + \pi_2(1-\alpha) &= \pi_1 \\ \pi_1\beta + \pi_3\beta &= \pi_2 \\ \pi_1(1-\alpha) + \pi_3(1-\beta) &= \pi_3\end{aligned} \tag{91}$$

The solutions that satisfy these limiting distribution equations are

$$\begin{aligned}\pi_0 &= \frac{\alpha\beta}{1+\beta-\alpha} \\ \pi_1 &= \frac{\beta(1-\alpha)}{1+\beta-\alpha} \\ \pi_2 &= \frac{\beta(1-\alpha)}{1+\beta-\alpha} \\ \pi_3 &= \frac{(1-\alpha)(1-\beta)}{1+\beta-\alpha}\end{aligned} \tag{92}$$

Therefore, this is the limiting distribution for this Markov chain.

What is the long-run probability of rain?

$$\pi_0 + \pi_2 = \frac{\alpha\beta + (1-\alpha)\beta}{1+\beta-\alpha} = \pi_R \tag{93}$$

3. Genetics.

Consider a population of diploid organisms (like you and me; everyone carries two copies of every gene) and a particular gene for which there are two possible variants A and a. Each person in the population has one of the pair of genes (genotypes) in the following table. Suppose the proportions of these gene pairs in the population at generation n are given below. Because no other

Genotype	Proportion
AA	p_n
Aa	q_n
aa	r_n

combinations are possible, we know $p_n + q_n + r_n = 1$. A fundamental result from genetics is the *Hardy-Weinberg Equilibrium*. It says that when

a. mates are selected at random,
b. each parent randomly transmits one of its genes to each o?spring, and
c. there is no selection,

then the genotype frequencies remain constant from generation to generation, so that

$$\begin{aligned} p_{n+1} &= p_n = p \\ q_{n+1} &= q_n = q \\ r_{n+1} &= r_n = r \end{aligned} \tag{94}$$

for all $n \geq 0$.

Under Hardy-Weinberg Equilibrium, the following identities are true

$$p = \left(p + \frac{q}{2}\right)^2 \quad , \quad r = \left(r + \frac{q}{2}\right)^2 \tag{95}$$

To prove these equations, note that the probability of generating genotype AA in the next generation is just the probability of independently selecting two A genes. The probability of selecting an A gene is

$$\begin{aligned} P(A) &= P(\text{pass on } A|\text{parent is } AA)P(\text{parent is } AA) \\ &\quad P(\text{pass on } A|\text{parent is } Aa)P(\text{parent is } Aa) \\ &= 1 \times p \times \frac{1}{2} \times q \end{aligned} \tag{96}$$

Therefore, the probability of AA in next generation is

$$\left(p + \frac{q}{2}\right)^2$$

Finally, since the genotype frequencies are not changing across generations, the first equation is proven. The second equation can be shown in a similar fashion.

Now, construct the following Markov chain. Suppose that the chain starts with one individual of arbitrary genotype. This parent gives birth to one o?spring, which in turn gives birth to another o?spring. The state space consists of the three possible genotypes AA, Aa, aa of the long chain of offspring resulting from the original parent. The Markov matrix is given by

$$P = \begin{array}{c} \\ AA \\ Aa \\ aa \end{array} \begin{array}{c} \begin{array}{ccc} AA & Aa & aa \end{array} \\ \left\| \begin{array}{ccc} p + \frac{q}{2} & r + \frac{q}{2} & 0 \\ \frac{1}{2}\left(p + \frac{q}{2}\right) & \frac{1}{2} & \frac{1}{2}\left(r + \frac{q}{2}\right) \\ 0 & p + \frac{q}{2} & r + \frac{q}{2} \end{array} \right\| \end{array} \tag{97}$$

The limiting distribution of this process is $\pi = (p, q, r)$. To show this, we need only show that π satisfies the two equations from the theorem.

By definition

$$p + q + r = 1 \tag{98}$$

In addition, we must have

$$
\begin{aligned}
p &= p\left(p + \frac{q}{2}\right) + \frac{q}{2}\left(p + \frac{q}{2}\right) = \left(p + \frac{q}{2}\right)^2 \\
r &= r\left(r + \frac{q}{2}\right) + \frac{q}{2}\left(r + \frac{q}{2}\right) = \left(r + \frac{q}{2}\right)^2
\end{aligned} \tag{99}
$$

but by the Hardy-Weinberg equilibrium, these equations are true and the result is proven.

E. Techniques.

1. Determining the rate of transition between classes of states.

   a. If you want to calculate the rate of transition from state i to j in the long-run, you need to calculate

   $$P(X_n = i, X_{n=1} = j) = P(X_{n+1} = j | X_n = i) P(X_n = i) = p_{ij}\pi_i \tag{100}$$

   where n is sufficiently long that the long-run behavior of the chain applies (independence from initial state has been achieved).

   b. Suppose you have a Markov chain with two subsets of states, those that are Good (subset G) and those that are Bad (subset B).

   To calculate the rate of transition from Good states to Bad states, we merely sum over all possible combinations of good and bad states (the combinations are disjoint).

   $$P(X_n \in G, X_{n+1} \in B) = \sum_{i \in G} \sum_{j \in B} p_{ij}\pi_i \tag{101}$$

   c. **Example 1:** Verify that the proposed stationary distribution for the two- day weather model are the rates of transition, such that $\pi_0 = P(X_{n-1} = R, X_n = R)$, etc.

   d. **Example 2:** Suppose a manufacturing process changes state according to a Markov chain with transition probability matrix

   $$P = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & 0 & \frac{1}{2} \end{pmatrix} \tag{102}$$

Suppose further that states 0 and 1 are running states, but states 2 and 3 are down states. What is the breakdown rate?

We seek the rate at which the system transitions from states 0 or 1 to states 2 or 3

$$P(X_{n+1} = 2 \cup X_{n+1} = 3 | X_n = 0 \cup Xn = 1) = P(X_{n+1} \in B | X_n \in G) \tag{103}$$

where $B = \{2,3\}$ and $G = \{0,1\}$. First, we need the limiting distribution that satisfies the equations

$$\begin{aligned} \tfrac{1}{4}\pi_0 + \tfrac{1}{4}\pi_1 + \tfrac{1}{2}\pi_2 &= \pi_0 \\ \tfrac{1}{4}\pi_1 + \tfrac{1}{2}\pi_2 + \tfrac{1}{4}\pi_3 &= \pi_1 \\ \tfrac{1}{4}\pi_0 + \tfrac{1}{4}\pi_1 + \tfrac{1}{4}\pi_2 + \tfrac{1}{4}\pi_3 &= \pi_2 \\ \tfrac{1}{4}\pi_0 + \tfrac{1}{4}\pi_1 + \tfrac{1}{2}\pi_3 &= \pi_3 \end{aligned} \tag{104}$$

and has solution

$$\pi_0 = \tfrac{3}{16} \quad , \quad \pi_1 = \tfrac{1}{4} \quad , \quad \pi_2 = \tfrac{7}{24} \quad , \quad \pi_3 = \tfrac{13}{48} \tag{105}$$

The breakdown rate is

$$\begin{aligned} P(X_{n+1} \in B | X_n \in G) &= \pi_0 p_{02} + \pi_0 p_{03} + \pi_1 p_{12} + \pi_1 p_{03} \\ &= \frac{3}{16}\left(\frac{1}{2} + 0\right) + \frac{1}{4}\left(\frac{1}{2} + \frac{1}{4}\right) \\ &= \frac{9}{32} \end{aligned} \tag{106}$$

2. Average cost/earning per unit time.

Suppose there is a cost or a reward associated with each state in the Markov chain. We might be interested in computing the average earnings or cost of the chain over the long-run. We do so by computing the average long-term cost/value per time step.

a. **Proposition:** Let $\{X_n, n \geq 0\}$ be an irreducible Markov chain with stationary distribution $\pi_j, j \geq 0$ and let $r(i)$ be a bounded function on the state space. With probability 1

$$\lim_{N \to \infty} \frac{\sum_{n=0}^{N} r(X_n)}{N} = \sum_{j=0}^{\infty} r(j)\pi_j \tag{107}$$

Proof: Let $a_J(N)$ be the amount of time the Markov chain spends in state j up until time N. Then,

$$\sum_{n=1}^{N} r(X_n) = \sum_{j=0}^{\infty} a_j(N) r(j) \tag{108}$$

But, $\frac{a_j(N)}{N} \to \pi_j$, thus the result follows by dividing by N and letting $N \to \infty$.

b. **Example:** Suppose in the manufacturing example above that state 0 is highly productive, producing 100 units per day, state 1 is somewhat productive, producing 50 units per day, state 2 is somewhat costly, costing the equivalent of -10 units per day and state 3 is very costly, costing -20 units per day. What is the average daily earnings?

In this case,

$$r(0) = 100\ ,\ r(1) = 50\ ,\ r(2) = -10\ ,\ r(3) = -20$$

and the answer is

$$\sum_{i=0}^{3} r(i)\pi_j = \frac{100 \times 3}{16} + \frac{50 \times 1}{4} + \frac{14 \times (-10)}{48} + \frac{13 \times (-20)}{48} = 22.92$$

12 Basic Limit Theorem of Markov Chains

A. **Definition:** The *first return time* of a Markov chain is

$$R_i = \min_{n \geq 1} \{X_n = i\} \tag{109}$$

the first time the chain enters state i.

B. Let f_{ii}^n be the probability distribution of the first return time, hence

$$f_{ii}^n = P(R_i = n | X_0 = i) \tag{110}$$

For recurrent states, the chain is guaranteed to return to state i: $f_i = \sum_n f_{ii}^n = 1$.

For transient states, this is not a probability distribution since $\sum_n f_{ii}^n < 1$

C. The mean duration between visits to recurrent state i is given by

$$m_i = E[R_i | X_0 = i] = \sum_{n=1}^{\infty} n f_{ii}^n \tag{111}$$

D. **Definition:** State i is said to be *positive recurrent* if $m_i < \infty$. Otherwise, it is *null recurrent*. The distinction is only possible for infinite state Markov chains. All recurrent states in a finite state Markov chain are positive recurrent.

E. **Theorem:** Consider a recurrent, irreducible, aperiodic Markov chain. Then,

$$\lim_{n\to\infty} p_{ii}^n = \frac{1}{\sum_{n=0}^{\infty} n f_{ii}^n} = \frac{1}{m_i} \tag{112}$$

and $\lim_{n\to\infty} p_{ji}^n = \lim_{n\to\infty} p_{ii}^n$ for all states j.

Justification: The MC returns to state i on average every m_i steps. Therefore, it spends, on average, one in every m_i time steps in state i. The long-run proportion of time spent in i is

$$\pi_i = \frac{1}{m_i} \tag{113}$$

Of course, $\lim_{n\to\infty} p_{ii}^n = \lim_{n\to\infty} p_{ji}^n = \pi_i$ for irreducible, ergodic Markov chains. This "justification" fails to show that the above result also applies to null recurrent, irreducible, aperiodic Markov chains (i.e., not quite ergodic Markov chains).

F. **Lemma:** The theorem applies to any aperiodic, recurrent class C.

Proof: Because C is recurrent, it is not possible to leave class C once in one of its states. Therefore, the submatrix of P referring to this class is the transition probability matrix of an irreducible, aperiodic, recurrent MC and the theorem applies to the class.

G. **Lemma:** The equivalent result for a periodic chain with period d is

$$\lim_{n\to\infty} p_{ii}^{nd} = \frac{d}{m_i} \tag{114}$$

and

$$\lim_{n\to\infty} \frac{1}{n} \sum_{l=0}^{n-1} p_{ii}^l = \pi_i = \frac{1}{m_i} \tag{115}$$

$$\lim_{n\to\infty} \frac{1}{n} \sum_{l=0}^{n-1} p_{ki}^l = \pi_i = \frac{1}{m_i} \quad \text{for all states } k \neq i \tag{116}$$

H. Finding Patterns in Markov-Chain Generated Data

1. General Solution.

Consider a Markov chain $\{X_n, n \geq 0\}$ with transition probabilities p_{ij}. Suppose $X_0 = r$. What is the expected time until pattern $i_0, i_1, ..., i_k$ observed in the Markov chain realization?

Let

$$N(i_1, ..., i_k) = \min\{n \geq k : X_{n-k+1} = i_1, ..., X_n = i_k\} \tag{117}$$

Note that if $r = i_i$, we cannot count r as part of the matching pattern. Given this definition, we seek

$$E[N(i_1, ..., i_k)|X_0 = r] \tag{118}$$

Define a k-chain from the original Markov chain $\{X_n, n \geq 0\}$.

$$Z_n = (X_{n-k+1}, X_{n-k+2}, ..., X_n) \tag{119}$$

and let $\pi(j_1, ..., j_k)$ be the stationary probabilities of this k-chain. We know

$$\pi(j_1, ..., j_k) = \pi_{j_1} p_{j_1 j_2} p_{j_2 j_3} \cdots p_{j_{k-1} j_k} \tag{120}$$

by our work with long-run unconditional probabilities. Our new results indicate

$$m_{i_1 i_2 \cdots i_k} = \frac{1}{\pi(i_1, ..., i_k)} \tag{121}$$

We need to consider whether or not there is an overlap in the pattern.

Definition: Pattern $i_1, ..., i_k$ has overlap of size $j < k$ if $(i_{k-j+1}, i_{k-j+2}, ..., i_k) = (i_1, ..., i_j)$ for $j < k$.

Case 1: no overlap.

$$\begin{aligned} E[Z_n = (i_1, ..., i_k)|Z_0 = (i_1, ..., i_k)] &= E[N(i_1, ..., i_k)|X_0 = i_k] \\ &= \frac{1}{\pi(j_1, ..., j_k)} \end{aligned} \tag{122}$$

but

$$E[N(i_1, ..., i_k)|X_0 = i_k] = W_{i_k i_1} + E[A(i_1)] \tag{123}$$

where $A(i_1)$ is the number of steps required to match the pattern given that i_1 has currently been matched and the $W_{i_k i_1}$ are the expected wait times until absorption into state i_1 from i_k, in this case it is the expected time until state i_1 is first hit given the chain starts in i_k. The above equation, gives us an expression for $E[A(i_1)]$, which we utilize in

$$\begin{aligned} E[N(i_1, ..., i_k)|X_0 = r] &= W_{ri_1} + E[A(i_1)] \\ &= W_{ri_1} + \frac{1}{\pi(i_1, ..., i_k)} - W_{i_k i_1} \end{aligned} \tag{124}$$

Case 2: overlap. Let the largest overlap have length s. Suppose we have just matched the pattern. Then we are s steps into a potential new match. We have,

$$\begin{aligned} E[N(i_1, ..., i_k)|X_{-s+1} = i_1, X_{-s+2} = i_2, ..., X_0 = i_s] &= \frac{1}{\pi(i_1, ..., i_k)} \\ &= E[A(i_1, ..., i_s)] \end{aligned} \tag{125}$$

In addition, because $N(i_1, ..., i_k) = N(i_1, ..., i_s) + A(i_1, ..., i_s)$, we have

$$E[N(i_1, ..., i_k)|X_0 = r] = E[N(i_1, ..., i_s)|X_0 = r] + E[A(i_1, ..., i_s)|X_0 = r] \tag{126}$$

but

$$\begin{aligned} E[A(i_1, ..., i_s)|X_0 = r] &= E[A(i_1, ..., i_s)] \\ &= \frac{1}{\pi(i_1, ..., i_k)} \end{aligned} \tag{127}$$

One then repeats the whole procedure for pattern $i_1, ..., i_s$ until a pattern with no overlaps is found and procedure 1 can be applied.

2. Example: pattern matching.

   What is the expected time before the pattern 1,2,3,1,2,3,1,2 is achieved given $X_0 = r$? The maximum overlap is of length $s = 5$.

$$\begin{aligned}
E[N(1,2,3,1,2,3,1,2)|X_0 = r] &= E[N(1,2,3,1,2)|X_0 = r] \\
&\quad + \frac{1}{\pi(1,2,3,1,2,3,1,2)} \\
E[N(1,2,3,1,2)|X_0 = r] &= E[N(1,2)|X_0 = r] \\
&\quad + \frac{1}{\pi(1,2,3,1,2)} \\
E[N(1,2)|X_0 = r] &= W_{r1} + \frac{1}{\pi_i(12)} - W_{21} \qquad (128)
\end{aligned}$$

   Working our way back up the equalities and substituting in expressions for $\pi(\cdot)$ we have

$$\begin{aligned}
E[N(1,2)|X_0 = r] &= W_{r1} + \frac{1}{\pi_1 p_{12}} - W_{21} \\
&\quad + \frac{1}{\pi_1 p_{12}^2 p_{23} p_{31}} + \frac{1}{\pi_1 p_{12}^3 p_{23}^2 p_{31}^2} \qquad (129)
\end{aligned}$$

3. Special case: iid random variables.

   If the Markov chain is generated by iid random variables, then the transition probabilities are

$$p_{ij} = P(X_n = j|X_{n-1} = i) = P(X_n = j) = p_j \qquad (130)$$

   i.e., all rows of the transition probability matrix are identical.

   In this case, the time between visits to a state i is a geometric random variable with mean $W_{ii} = \frac{1}{p_i}$. In this special case, the expected time to the above pattern is

$$E[N(1,2,3,1,2,3,1,2)|X_0 = r] = \frac{1}{p_1 p_2} + \frac{1}{p_1^2 p_2^2 p_3} + \frac{1}{p_1^3 p_2^3 p_3^2} \qquad (131)$$

13 Reversed and Time-Reversible Markov Chains

A. A chain whose initial state distribution is equal to its stationary distribution or a chain that has run an infinite amount of time is said to be a "stationary Markov chain." It is said to have reached "stationarity."

B. Note, a time inhomogeneous Markov chain cannot reach stationarity. Only time homogeneous chains can run at stationarity.

C. The reversed Markov chain.

1. **Definition:** Assume we have a stationary, ergodic Markov chain with transition probability matrix P and stationary distribution π_i. Consider the chain in reverse, for example $X_{m+1}, X_m, X_{m-1}, X_{m-2}, \ldots$ This is called the *reversed chain*.
2. **Claim:** The reversed chain is also a Markov chain.

   Proof: The result is trivially realized. Consider a portion of the forward Markov chain

   $$\ldots, X_{m-2}, X_{m-1}, X_m, X_{m+1}, X_{m+2}, X_{m+3}, \ldots$$

   and suppose that X_{m+1} is the present state. Then, by the Markov property for the forward chain, the future $X_{m+2}, X_{m+3}, \ldots$ is independent of the past $\ldots, X_{m-1}, X_m$. But independence is a symmetric property, i.e., if X is independent of Y, then Y is independent of X, therefore the past $\ldots, X_{m-1}, X_m$ is independent of the future $X_{m+2}, X_{m+3}, \ldots$ In terms of the reversed chain, we then have that the past is independent of the future:

   $$P(X_m = j | X_{m+1} = i, X_{m+2}, \ldots) = P(X_m = j | X_{m+1} = i) \equiv q_{ij} \quad (132)$$

3. Transition probabilities of the reversed Markov chain.

   $$\begin{aligned} q_{ij} &= P(X_m = j | X_{m+1} = i) \\ &= \frac{P(X_m = j | X_{m+1} = i)}{P(X_{m+1} = i)} \\ &= \frac{\pi_j p_{ji}}{\pi_i} \end{aligned} \quad (133)$$

   where we have used the fact that the forward chain is running at stationarity.

D. Time-Reversible Markov Chain

1. **Definition:** time reversible Markov chain.

   An ergodic Markov chain is time reversible if $q_{ij} = p_{ij}$ for all states i and j.

2. **Lemma:** A Markov chain is time reversible if

$$\pi_i p_{ij} = \pi_j p_{ji} \tag{134}$$

   for all states i and j. Proof is obvious.

3. **Corollary:** If a Markov chain is time-reversible, then the proportion of transitions $i \to j$ is equal to the proportion of $j \to i$.

   Proof: To see this, note that the time reversibility condition given in the lemma is $P(X_n = i, X_{n+1} = j) = P(X_n = j, X_{n+1} = i)$ for any n sufficiently large that stationarity applies, but $P(X_n = i, X_{n+1} = j)$ is the proportion of transitions that move $i \to j$ and $P(X_n = j, X_{n+1} = i)$ is for transitions $j \to i$. Thus, the result is proved.

4. **Lemma:** If we can find π_i with $\sum_{i=0}^{\infty} \pi_i = 1$ and $\pi_i p_{ij} = \pi_j p_{ji}$ for all states i, j, then the process is reversible and π_i is the stationary distribution of the chain.

   Proof: Suppose we have x_i such that $\sum_{i=0}^{\infty} x_i = 1$. Then,

$$\sum_{i=0}^{\infty} x_i p_{ij} = \sum_{i=0}^{\infty} x_j p_{ji} = x_j \sum_{i=0}^{\infty} p_{ji} = x_j \tag{135}$$

   So, we have shown that the x_j satisfy the equations defining a stationary distribution and we are done.

5. **Example:** Consider a random walk on the finite set $0, 1, 2, ..., M$. A random walk on the integers (or a subset of integers, as in this case) moves either one step left or one step right during each timestep. The transition probabilities are

$$\begin{aligned} p_{i,i+1} &= \alpha_i = 1 - p_{i,i-1} \\ p_{0,1} &= \alpha_0 = 1 - p_{0,0} \\ p_{M,M} &= \alpha_M = 1 - p_{M,M-1} \end{aligned} \tag{136}$$

We argue that the random walk is a reversible process. Consider a process that jumps right from position $0 < i < M$, then if it is to jump right from i once again, it had to have jumped left from $i+1$ since there is only one way back to state i and that is via $i+1$. Therefore, for each jump right at i, there must have been a jump left from $i+1$. So, the fluxes (rates) left and right across the $i \leftrightarrow i+1$ boundary are equal. (Note, this argument is not fully rigorous.)

Since the process is time-reversible, we can obtain the stationary distribution from the reversibility conditions

$$\begin{aligned} \pi_0\alpha_0 &= \pi_1(1-\alpha_1) \\ \pi_1\alpha_1 &= \pi_2(1-\alpha_2) \\ \vdots &= \vdots \\ \pi_i\alpha_i &= \pi_{i+1}(1-\alpha_{i+1}) \\ \vdots &= \vdots \\ \pi_{M-1}\alpha_{M-1} &= \pi_M(1-\alpha_M) \end{aligned} \tag{137}$$

with solution

$$\begin{aligned} \pi_1 &= \frac{\alpha_0\pi_0}{1-\alpha_1} \\ \pi_2 &= \frac{\alpha_1\alpha_0\pi_0}{(1-\alpha_2)(1-\alpha_1)} \\ \vdots &= \vdots \end{aligned} \tag{138}$$

Then use the condition $\sum_{i=0}^{M}\pi_i = 1$ to find that

$$\pi_0 = \left[1 + \sum_{j=1}^{M} \frac{\alpha_{j-1}\cdots\alpha_0}{(1-\alpha_j)\cdots(1-\alpha_1)}\right]^{-1} \tag{139}$$

6. **Theorem:** An ergodic MC with $p_{ij} = 0$ whenever $p_{ji} = 0$ is time reversible if and only if any path from state i to state i has the same probability as the reverse path. In other words,

$$p_{ii_1}p_{i_1i_2}\cdots p_{i_ki} = p_{ii_k}p_{i_ki_{k-1}}\cdots p_{i_1i} \tag{140}$$

for all states $i, i_1, ..., i_k$ and integers k.

Proof: Assume reversibility, then

$$\begin{aligned}\pi_i p_{ij} &= \pi_j p_{ji} \\ \pi_k p_{kj} &= \pi_j p_{jk} \\ \pi_i p_{ik} &= \pi_k p_{ki}\end{aligned} \tag{141}$$

Using the first two equations we obtain an expression for

$$\frac{\pi_i}{\pi_k} = \frac{p_{ji} p_{kj}}{p_{jk} P_{ij}} \tag{142}$$

Another expression for this ratio is obtained from the third equation

$$\frac{\pi_i}{\pi_k} = \frac{p_{ki}}{P_{ik}} \tag{143}$$

Equating these two expressions for the ratio, we obtain

$$p_{ij} p_{jk} P_{kj} = p_{ik} p_{kj} p_{ji} \tag{144}$$

implying that the path $i \to j \to k \to i$ has the same probability as the reverse path $i \to k \to j \to i$. The argument given here can be extended to arbitrary paths between arbitrary states.

To show the converse, we assume that

$$p_{ii_1} p_{i_1 i_2} \cdots p_{i_k j} p_{ji} = p_{ij} p_{j i_k} p_{i_k i_{k-1}} \cdots p_{i_1 i} \tag{145}$$

then sum over all possible intermediate states in the path

$$\sum_{i_i, i_2, \ldots, i_k} p_{ii_1} p_{i_1 i_2} \cdots p_{i_k j} p_{ji} = \sum_{i_i, i_2, \ldots, i_k} p_{ij} p_{j i_k} p_{i_k i_{k-1}} \cdots p_{i_1 i} \tag{146}$$

$$p_{ij}^{(k+1)} p_{ji} = p_{ij} P_{ji}^{(k+1)} \tag{147}$$

Now, let $k \to \infty$, then the $(k+1)$-step transition probabilities converge to the limiting distribution and we obtain

$$\pi_j p_{ji} = \pi_i p_{ij} \tag{148}$$

which shows time reversibility.

14 Markov Chain Monte Carlo

Let X be a discrete random vector with values $x_j, j \geq 1$ and pmf(probability mass function) $P(X = x_j)$. Suppose we want to estimate $\theta = E[h(X)] = \sum_{j=1}^{\infty} h(x_j)P(X = x_j)$.

If $h(x)$ is difficult to compute, the potentially infinite sum on the right can be hard to compute, even approximately, by slowly iterating over all possible x_j.

A. **Monte Carlo Simulation:** In Monte Carlo simulation, an estimate of θ is obtained by generating $X_1, X_2, ..., X_n$ as independent and identically distributed random variables from pmf $P(X = x_j)$. The Strong Law of Large Numbers shows us that

$$\lim_{n\to\infty} \sum_{i=1}^{n} \frac{h(x_i)}{n} = \theta \tag{149}$$

So we as we generate $X_1, X_2, ...,$ compute $h(X_1), h(X_2), ...$ and average the resulting numbers, that value will be a better and better approximation of θ as n grows large.

B. **The Need for Markov Chain Monte Carlo:** Suppose it is difficult to generate iid X_i or that the pmf is not known and only b_j are known such that

$$P(X = x_j) = Cb_j \tag{150}$$

where C is an unknown constant, i.e., you know the "pmf up to a constant".

To solve this problem we will generate the realization of a Markov chain $X_1, X_2, ..., X_n$ where the X_i are no longer iid, but come instead from a Markov chain. A previous result we have shown indicates that

$$\lim_{n\to\infty} \sum_{i=1}^{n} \frac{h(X_i)}{n} = \sum_{j=1}^{\infty} h(j)\pi_j \tag{151}$$

so if $\pi_j = P(X = x_j)$, then the same average we computed in Monte Carlo simulation will still be an estimate of θ. In other words, if we could construct a Markov chain with stationary distribution $\pi_j = P(X = x_j)$ and we generated a realization $X_1, X_2, ...$ of that Markov chain, evaluated $h(\cdot)$ at each state of the chain $h(X_1), h(X_2), ...$ and computed the average of these numbers, it will provide an estimate of θ.

C. **Metropolis-Hastings Algorithm - A Special Implementation of MCMC** Assume $\sum_{j\geq 1} b_j < \infty$, then the following is a procedure for generating a Markov Chain on the sample space of X with transition probability matrix (tpm) $P = (p_{ij})$ matching the criteria above. The Markov chain must be recurrent and irreducible so that the stationary distribution exists and that stationary distribution should satisfy $\pi_j = P(X = x_j)$ so that the above estimation procedure works.

Let Q be any transition probability matrix of any irreducible Markov chain on the state space of X. It has transition probabilities q_{ij}.

Suppose the current state of the P MC is $X_n = i$. Then, the algorithm proceeds as follows:

1. Generate a random variable $Y = j$ with probability q_{ij} according to the Q MC.
2. Set the next state in the P MC to

$$X_{n+1} = \begin{cases} j & \text{with probability } \alpha_{ij} \\ i & \text{with probability } 1 - \alpha_{ij} \end{cases} \tag{152}$$

where

$$\alpha_{ij} = \min\left\{\frac{\pi_j q_{ji}}{\pi_i q_{ij}}, 1\right\} \tag{153}$$

Note, that while we do not actually know π_j, we know b_j and we have

$$\frac{\pi_j}{\pi_i} = \frac{b_j}{b_i} \tag{154}$$

Thus, we may compute

$$\alpha_{ij} = \min\left\{\frac{b_j q_{ji}}{b_i q_{ij}}, 1\right\} \tag{155}$$

as a function of parameters that are all known.

The above procedure induces the Markov chain with transition probability matrix P and entries

$$p_{ij} = \begin{cases} q_{ij}\alpha_{ij} & j \neq i \\ q_{ii} + \sum_{k\neq i} q_{ik}(1-\alpha_{ik}) & j = i \end{cases} \tag{156}$$

that defines how the realization $X_1, X_2, ...$ is generated.

We need to confirm that this MC with matrix P has the appropriate stationary distribution. The chain will be time-reversible with stationary distribution π_j if $\sum_j \pi_j = 1$ (this is given since the π_j are a pmt) and

$$\pi_i p_{ij} = \pi_j p_{ji} \tag{157}$$

for all $i \neq j$. But, according to the definitions of the transition probabilities this condition is

$$\pi_i q_{ij}\alpha_{ij} = \pi_j q_{ji}\alpha_{ji} \tag{158}$$

Suppose

$$\alpha_{ij} = \frac{\pi_j q_{ji}}{\pi_i q_{ij}}$$

Then,

$$\alpha_{ji} = \min\left\{\frac{\pi_i q_{ij}}{\pi_j q_{ji}}, 1\right\} = 1$$

Therefore, in this case,

$$\pi_i q_{ij}\frac{\pi_j q_{ji}}{\pi_i q_{ij}} = \pi_j q_{ji} = \pi_j q_{ji}\alpha_{ji} \tag{159}$$

since $\alpha_{ji} = 1$. Thus, we have shown the condition when $\alpha_{ij} = \frac{\pi_j q_{ji}}{\pi_i q_{ij}}$. It is straightforward to show the condition when $\alpha_{ij} = 1$ also.

At this point, we have shown that the constructed Markov chain has the desired stationary distribution π_j. Thus, random variables $X_1, X_2, ..., X_n$ generated according to this Markov chain will provide an estimate of θ via the Monte Carlo estimation formula.

D. **Example:**

Let $\mathcal{L}$ be the set of all permutations $x_j = (y_1, y_2, ..., y_n)$ of the integers $(1, 2, ..., n)$ such that $\sum_j j y_j > a$. We will use MCMC to generate $X \in \mathcal{L}$ with pmt $P(X = x_j)$ uniform over all permutations in $\mathcal{L}$. Because the target pmf is uniform, we have that $\pi_s = \frac{1}{|\mathcal{L}|}$ for all $s \in \mathcal{L}$, where $|\mathcal{L}|$ is the number of elements in the set $\mathcal{L}$.

We first need to define an irreducible MC with tpm Q. We can do this any way we would like. Define the neighborhood $N(s)$ of an element $s \in \mathcal{L}$ as all those permutations which can be obtained from s by swapping to numbers. For example (1,2,4,3,5) is a neighbor of (1,2,3,4,5), but (1,3,4,2,5) is not. Define the transition probabilities as

$$q_{st} = \frac{1}{|N(s)|} \tag{160}$$

where $|N(s)|$ is the number of permutations in the neighborhood of s. Therefore, the proposed permutation is equally likely to be any of the neighboring permutations. According the Metropolis-Hastings procedure, we define the acceptance probabilities as

$$\alpha_{st} = \min\left\{\frac{|N(s)|}{|N(t)|}, 1\right\} \tag{161}$$

where the π_s and the π_t cancel because they are equal. Note, with this, we are done constructing the transition probabilities p_{ij}.

What might be the advantage to developing such a procedure? It may be very difficult to sample random permutations that meet the criteria $\sum_j j y_j > a$, since very few of the $n!$ permutations may satisfy that criteria. The above procedure explores the permutation space in a methodical way and insures, in the long run, that each permutation in $\mathcal{L}$ is sampled with probability $\frac{1}{|\mathcal{L}|}$.

Suppose, for example, that you are interested in computing $E[\sum_{j=1}^n j y_j]$ for $x_j = (y_1, ..., y_n) \in \mathcal{L}$, that is the average value of $\sum_{j=1}^n j y_j$ given that $\sum_{j=1}^n j y_j > a$. You sample $X_1, X_2, ..., X_n$ from the above Markov chain as follows

1. Start in any state $X_0 = x_i$ in $\mathcal{L}$ (any convenient one you can find).
2. Suppose the current state is $X_n = x_j$.
3. Compute a list of permutations in the neighborhood $N(x_j)$ and generate a random number, let's say k, from the set $\{0, ..., |N(x_j)|\}$ to propose a new state from the Q chain. Suppose the kth member of $N(x_0)$ is x_l.
4. Compute $\alpha_{x_j x_l}$. Generate a random variable $U \sim \text{Unif}(0, 1)$. If $U < \alpha_{x_j x_l}$, then set $X_{n+1} = x_l$, otherwise set $X_{n+1} = x_j$.
5. Repeat N times to generate $X_0, X_1, ..., X_N$, where N is big enough to insure the estimate converges.
6. Compute $h(X_0), h(X_1), ..., h(X_N)$ and compute the estimate

$$\hat{\theta} = \frac{1}{N} \sum_{n=1}^{N} h(X_n) \tag{162}$$