DATA 581

Modeling and Simulation II

Lecture 5: Markov Chain Models

What We Discuss Today

- Mouse Movement Example
- Descrete Time Markov Chains
- Simulating from a Markov Chain Model
- Stationary Distribution

It only matters where you are, not where you have been!

- Markov chain is named after a Russian Mathematician, ***Andrey Markov***.

- They have been used in many different domains, ranging from text generation to financial modeling and weather forecasting.

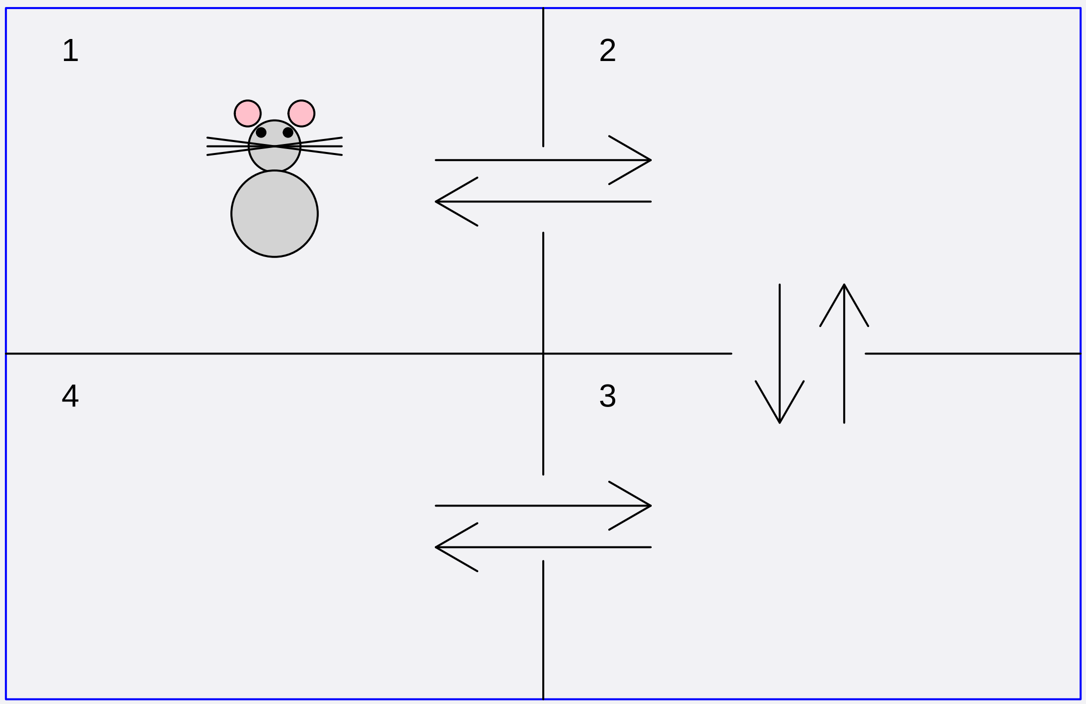
- Generally, any system that experiences transitions from one state to another according to certain probabilistic rules.

- two different types of Markov chain:
  - discrete-time Markov chains; where the changes happen at specific states
  - continuous-time Markov chains; where the changes are continuous.

Example

- We begin with an example that illustrates many of the concepts that arise when studying and simulating from Markov chain models.
- A four-compartment maze in which a mouse can wander between compartments as indicated by the directions of the arrows.

A Mouse in a Maze



Mouse movement Model - Complete Randomness

The location or state of the mouse at the time immediately after the n-th move is recorded as X_n.

For example, if the mouse starts in compartment 1, and enters compartment 2, then compartment 3, back to 2, back to 3, then 4, and back to 3, and so on, we write this as;

$$X_0 = 1, X_1 = 2, X_2 = 3, X_3 = 2, X_4 = 3, X_5 = 4, X_6 = 3, \ldots.$$

Question: How did we obtain the above path (trajectory) for the mouse movement model?

The pattern in this kind of random (or more learnedly, stochastic) sequence is governed, in part, by transition rules that follow from model assumptions.

Mouse movement Model - Transition probabilities

For our example, let's assume complete randomness: the mouse is moving in random directions, stopped only by the compartment walls.

To calculate the transition probability that the mouse would enter compartment 2, given that the mouse is currently in compartment 1, we observe that there is no other possible transition for the mouse. If the mouse is moving at random, eventually, the mouse will find the passageway to compartment 2, and we would conclude that the transition probability from compartment 1 to compartment 2 is exactly 1.0.

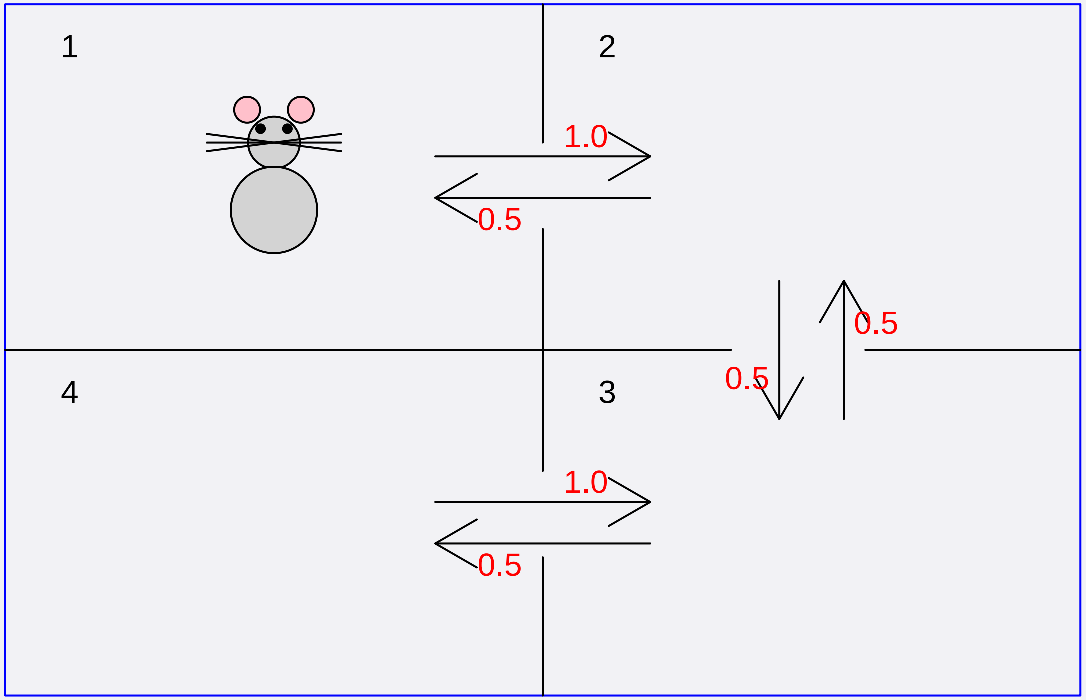
$$P(X_1 = 2|X_0 = 1) = 1$$

Once in compartment 2, the mouse could possibly return to compartment 1, but it is equally likely to find the passageway to compartment 3. Therefore, the transition probabilities from compartment 2 to compartments 1 and compartments 3 are both 0.5. It is not possible for the mouse to travel directly to compartment 4, so this transition probability is 0.

$$P(X_2 = 3|X_1 = 2) = 0.5, P(X_2 = 1|X_1 = 2) = 0.5, P(X_3 = 3|X_2 = 1) = 0$$

A Mouse Movement Model - Transtition Probabilities

Transition Probabilities



Mouse movement Model - Transition matrix

The transition probabilities can be organized systematically into a matrix, noting that impossible transitions have probability 0.

The 1st row of the matrix lists the transition probabilities from the first compartment to all other compartments. We assume that the mouse is not staying in compartment 1: 0, 1, 0, 0.

2nd row – transition probabilities out of compartment 2: 0.5, 0, 0.5, 0.

3rd row – transition probabilities from compartment 3: 0, 0.5, 0, 0.5.

4th row – transition probabilities out of compartment 4: 0, 0, 1, 0.

Transition Matrix

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

Entry (i, j) represents the probability of transition into compartment j, given that the mouse was in state i.

We are assuming that p_{ij} does not depend on n.

All rows of P sum to one!

One important interpretation of this fact is that each row of a transition matrix is a probability distribution for a discrete random variable.

Some Terminology & Definitions

- **State Space (S): is the set of all possible states that a Markov chain can visit.**

- **A state space can be finite or infinite. where the individual states are often represented by the natural numbers.**
  - **The number of customers waiting for service from a corporate voice-messaging system is often modeled as a Markov chain. In theory, there is no bound on the number of customers in such a system, so the state space is $S = \{0, 1, 2, \ldots\}$.**

- **mouse movement example has a finite state $S = \{1, 2, 3, 4\}$.**

- **States do not have to be numeric, and in fact, the `factor()` object in R is perhaps the best way to think of the states of a Markov chain**

Some Terminology & Definitions

The sequence of random variables $X_1, X_2, X_3, \ldots,$ is called a Markov chain if

$$P(X_n = j_n | X_{n-1} = j_{n-1}, X_{n-2} = j_{n-2}, \ldots)$$

$$= P(X_n = j_n | X_{n-1} = j_{n-1})$$

where $j_n, j_{n-1}, j_{n-2}, \ldots$ are elements of S.

This is **Markov Property**.

This property states that the probability of the next state only depends on the current state, everything before the current state is irrelavent. In other words, the whole system is completely memoryless.

Simulating a finite state Markov chain

Using a sequence of independent uniform random numbers, we can simulate a Markov chain by using the probability distributions defined by the rows of the transition matrix.

Let's simulate a few transitions for the mouse movement model;

X_n **denotes the compartment holding the mouse at time** n**.**

Since the mouse starts in the first compartment, $X_0 = 1$**. At the first transition, the mouse enters the second compartment:** $X_1 = 2$ **with probability 1. At the second transition, the mouse can enter compartment 1 with probability 0.5 or compartment 3 with probability 0.5.**

To simulate the second transition, we need to generate a pseudorandom number which we will call U_2**. If** $U_2 < 0.5$**, we will make a rule that the mouse should enter compartment 1. Otherwise, it will enter compartment 3. If we obtain the value** $U_2 = 0.61$**, then the mouse enters the 3rd compartment:** $X_2 = 3$**.**

Simulating a finite state Markov chain

For the succeeding transitions, we continue generating uniform random variates, U, on the interval $[0, 1]$, choosing to move to the compartment labelled with the lower value if $U < 0.5$, and choosing to move to the higher valued compartment if $U \geq 0.5$, unless the mouse is already in compartment 4.

A possible sequence of U values is:

$U_3 = 0.34$, $U_4 = 0.88$, $U_5 = 0.52$.

Then the mouse locations are: $X_3 = 2$, $X_4 = 3$, $X_5 = 4$.

The mouse must re-enter compartment 3 with probability 1, so $X_6 = 3$,

Continuing in this way, we obtain the sequence of values of $\{X_1, X_2, X_3, \ldots\}$, which is an example of a Markov chain realization.

Simulating MC Model in R

Automating the Markov chain simulation process with R can be done in several ways.

A simple way to simulate values of X_j given the value of X_{j-1} is to use the `sample()` function.

Example: **simulating from a discrete probability distribution by setting the `prob` argument which specifies different probability weights for each possible value.**

$$P(X = 1) = 0.1, P(X = 2) = 0.2, P(X = 3) = 0.1, P(X = 4) = 0.4, P(X = 5) = 0.2$$

```
sample(1:5, size = 6, replace = TRUE,
       prob = c(.1, .2, .1, .4, .2))

## [1] 4 1 4 5 4 4
```

Simulating MC Model in R

Note: When simulating values in a Markov chain, we are simulating from probability distributions defined by the rows of the transition matrix.

Let's simulate 10000 moves from the mouse movement markov chain starting from compartment 1.

```
Ntransitions <- 10000 # number oftransitions
P <- matrix(c(0, 1, 0, 0,
              0.5, 0, 0.5, 0,
              0, 0.5, 0, 0.5,
              0, 0, 1, 0), nrow = 4,
              byrow = TRUE)  # P is the transition matrix
X <- numeric(Ntransitions)#initializing the chain
current.state <- 1 # initial state X_0 = 1
for (t in 1:Ntransitions) {
  current.state <- sample(1:4,
       size = 1, prob = P[current.state, ])
  X[t] <- current.state
}
```

Simulating the Model in R

The first ten values of the simulation run are:

```
X[1:10]

##  [1] 2 1 2 3 2 3 4 3 4 3
```

It is useful to tabulate the results so that we can see the frequency of visits to the various states. (compartment)

We can count number of visits to each compartment by calling `table()`**.**

```
table(X)

## X
##    1    2    3    4
## 1679 3366 3321 1634
```

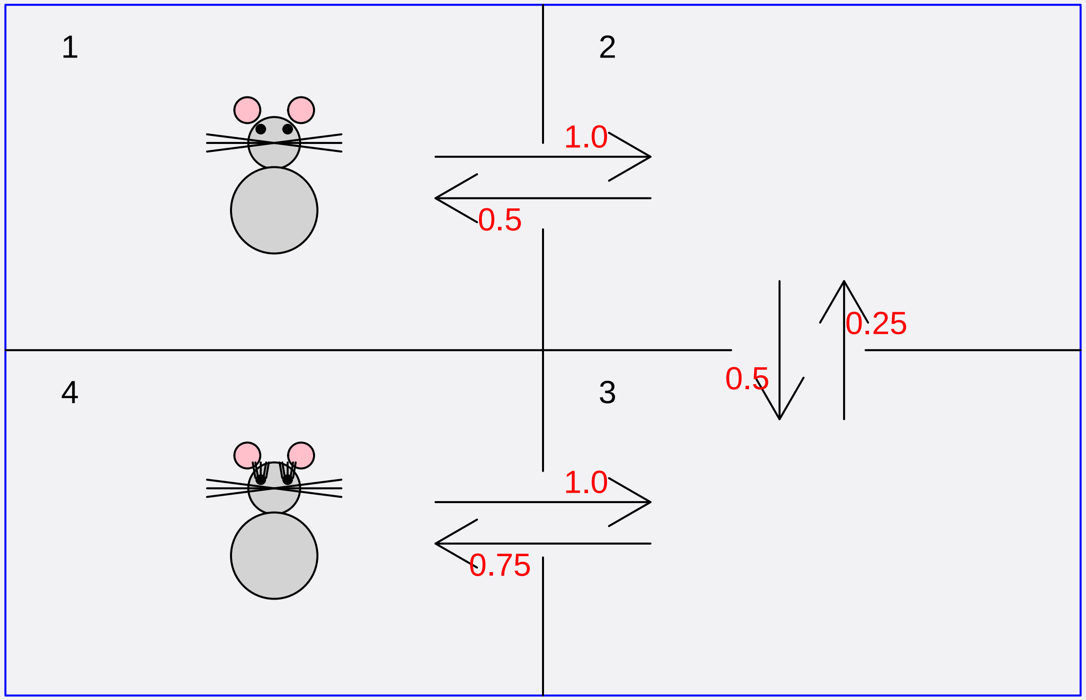
Also the relative frequency of the visits;

```
table(X)/Ntransitions

## X
##      1      2      3      4
## 0.1679 0.3366 0.3321 0.1634
```

A Mouse Movement Model - Including Some Structure

The transition probabilities for this experiment can be altered in other ways, possibly by including the odor of another mouse, usually of the opposite sex. .



A Mouse Movement Model - Some Structure

Transition Matrix

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.25 & 0 & 0.75 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Simulating the More Structured Model in R

Let’s simulate from this new model.

```r
Ntransitions <- 100000 # number of mouse moves
P <- matrix(c(0, 1, 0, 0,
              0.5, 0, 0.5, 0,
              0, 0.25, 0, 0.75,
              0, 0, 1, 0), nrow = 4,
              byrow = TRUE)  # P is the transition matrix
location <- numeric(Ntransitions)#initializing the Markov chain
current.state <- 1 # initial compartment
for (t in 1:Ntransitions) {
  current.state <- sample(1:4,
        size = 1, prob = P[current.state, ])
  location[t] <- current.state
}
table(location)/Ntransitions # the odor in compartment 4 is attractive

## location
##       1       2       3       4
## 0.10068 0.20074 0.39932 0.29926
```

The odor in compartment 4 is attractive, so the mouse makes more visits to that compartment than he would have when the odor is not present.

Stationary Distribution

- If we simulate this Markov chain for a long time, we will find that the proportions of visits to each location follows a specific distribution.

- This distribution is known as **stationary distribution**.

- In the null model with four compartments, the stationary distribution is

$$\frac{1}{6}, \frac{1}{3}, \frac{1}{3}, \frac{1}{6}$$

- In the model with the odor, the stationary distribution is different.

Some Theoritical Notes on Stationary Distribution

- **Remember in transition matrix P, entry (i, j) represents the probability of transition into state j, given that we were in state i.**

- **The transition, however, is only one-step.**

- **Question:** **How about a two-step journey from state i to j?**

- **The Chapman-Kolmogorov Equations:**
  - **if we wanted to calculate the n-step probabilities;**

$$P_{ij}^{n} = [P_{i}j]^{n}$$

  - **what would happen as n becomes large?**

More Notes on Stationary Distribution

- As we progress through time, we are more likely to be in certain states than others.
  - the probability of being in certain states are higher than others.

- Eventually, the distribution will reach an equilibrium and each state will be associated with a probability.

- The Stationary Distribution is the result of this process.

More Notes on Stationary Distribution

- **Why stationary? if you apply the Transition Matrix to this given distribution, the resultant distribution is the same as before.**

$$\pi = \pi P$$

- **In other words, over the long run, no matter what the starting state was, the proportion of time the chain spends in state j is approximately π_j for all j.**

- **The stationary distribution for mouse movement is $\pi = \left[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}, \frac{1}{6}\right]$.**

- **meaning over the long run; no matter where the mouse started,**
  - **mouse would be in compartment 1 with probability of $1/6 \approx 0.166$,**
  - **in comparment 2 with probability of $1/3 \approx 0.333$,**
  - **in comparment 3 with probability of $1/3 \approx 0.333$,**
  - **in comparment 4 with probability of $1/6 \approx 0.166$,**

- **familiar? simualted from the model and after 100000 moves the relative frequency of each state was:**

```
table(X)/Ntransitions

## X
##       1       2       3       4
## 0.01679 0.03366 0.03321 0.01634
```

What to Take Away From Today's Lecture

- Markov chain property
- Discrete Time Markov Model
- Stationary Distribution