Chapter 2 - Simulating Statistical Models

Markov Chains.

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Stochastic Process

Definition
A **stochastic process** is a collection of random variables

$$X = \{X_t\}_{t \in T}, \quad X_t \in S$$

where

- T = **index set** (often time: $\mathbb{N}$ for discrete, $\mathbb{R}^+$ for continuous)
- S = **state space** (possible values of X_t)

Examples

- Tossing a coin repeatedly: $X_t \in \{0, 1\}$
- Daily stock price: $X_t \in \mathbb{R}^+$
- Temperature over time: $X_t \in \mathbb{R}$

Key Idea

The random variables X_t are usually **dependent**, and interesting processes have *structured dependence*.

Dependence Structure

Classical Assumption
Many results in probability theory assume that random variables are **independent**, which makes computations much easier.

But in Reality...

- Independence is often **not realistic** (e.g., stock prices, weather, genetics).
- Random variables are usually **dependent**.

The Challenge

Therefore, adding dependence between random variables makes computations more difficult.

Goal: Find dependence structures that are both **realistic and computationally workable**.

BEHOLD: The most awesome Markov Chains

They provide a simple yet powerful model of dependence: the future depends only on the present, not on the entire past.

Dependence in a Markov Chain

Intuition

A Markov chain has **no memory**. That is to say that the **most recent state** only matters for predicting the next one.

Definition 1 (Discrete-Time Markov Chain)

A stochastic process

$$X = \{X_0, X_1, X_2, \ldots\}, \quad X_n \in S$$

satisfies the **Markov property** if for all $n \geq 0$,

$$P(X_{n+1} \in A_j \mid X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n) = P(X_{n+1} \in A_j \mid X_n = i_n).$$

Notes

- The distribution of X_0 is called the **initial distribution**.
- Sometimes X_0 is known (and not random).
- The condition above is called the **Markov property**, named after Russian mathematician Andrey Markov.

Simple random walk

Let $\{Y_k\}_{k\geq 1}$ be i.i.d. random variables ("steps") with

$$\mathbb{P}(Y_k = 1) = p, \qquad \mathbb{P}(Y_k = -1) = 1 - p$$

Fix an initial state $X_0 \in \mathbb{Z}$. Define the *random walk*

$$X_n = X_0 + \sum_{k=1}^{n} Y_k, \qquad n \geq 1$$

Thus each step moves the walker by $+1$ or -1.

Intuition
The next position X_{n+1} is obtained by adding one fresh independent step Y_{n+1} to the current position X_n.

Proposition 1
The random walk $\{X_n\}$ defined above satisfies the Markov property: for all $n \geq 0$ and integers $i_0, \ldots, i_n, j$,

$$\mathbb{P}(X_{n+1} = j \mid X_0 = i_0, \ldots, X_n = i_n) = \mathbb{P}(X_{n+1} = j \mid X_n = i_n)$$

Random Walk $\Rightarrow$ Markov Property (example-based proof)

Proof. Start from the left-hand conditional probability and use the construction $X_{n+1} = X_n + Y_{n+1}$:

$$\begin{aligned}\mathbb{P}(X_{n+1} = j \mid X_0 = i_0, \ldots, X_n = i_n) &= \mathbb{P}(i_n + Y_{n+1} = j \mid X_0 = i_0, \ldots, X_n = i_n) \\ &= \mathbb{P}(Y_{n+1} = j - i_n \mid X_0 = i_0, \ldots, X_n = i_n).\end{aligned}$$

Because Y_{n+1} is independent of the past (the $\{Y_k\}$ are i.i.d.), the conditioning on $X_0, \ldots, X_n$ is irrelevant, so

$$\mathbb{P}(Y_{n+1} = j - i_n \mid X_0, \ldots, X_n) = \mathbb{P}(Y_{n+1} = j - i_n).$$

Why the Markov Property Holds (Random Walk Example)

The event $\{X_{n+1} = j\}$ is the same as

$$\{ i_n + Y_{n+1} = j \} \quad \Longleftrightarrow \quad \{ Y_{n+1} = j - i_n \}$$

Thus,

$$\mathbb{P}(X_{n+1} = j \mid X_n = i_n) = \mathbb{P}(Y_{n+1} = j - i_n)$$

Since Y_{n+1} is independent of the past, the history $(X_0, \ldots, X_{n-1})$ does not matter. Hence the Markov property holds all $n \geq 0$ and integers $i_0, \ldots, i_n, j$.

Why the Markov Property Holds – Example

A Gambler's Fortune. Let X_n be the amount of money a gambler has after n bets. At each step:

$$X_{n+1} = X_n + Y_{n+1}, \quad Y_{n+1} = \begin{cases} \text{heads} & \text{(win \$1)} \\ \text{tails} & \text{(lose \$1)} \end{cases}$$

If the gambler currently has \$10, then the next outcome depends only on the result of the next bet (Y_{n+1}), not on how they got to \$10.

But we can still see that for an unbiased coin ($p = \frac{1}{2}$)

$$P(X_n > 10) = \sum_{k=\lfloor n/2 \rfloor + 1}^{n} \binom{n}{k} \left(\frac{1}{2}\right)^n; \quad P(X_n > 10) \approx \frac{1}{2} \quad \text{as } n \to \infty\text{; by CLT}$$

Takeaway
The process is Markov because the *future fortune depends only on the present fortune and the next bet*, not the entire betting history.

Markov Property Discussion

Interpretation: The future is independent of the past given the present.

- Natural in many applications:
  - Total gains/losses in gambling
  - Cumulative processes such as queues
- The Markov property makes probability calculations much easier:
  - Compute probabilities and expectations step by step
  - No need to assume all random variables are independent

Homogeneous Markov Chain

Let us consider first the case of finite/discrete state space S.

Conditional probabilities of the type $P(X_{n+1} = j | X_n = i)$ are called one-step transition probabilities **from state i to state j**.

If these one-step transition probabilities do not depend on time variable n, then we say that the Markov Chain is **homogeneous** and we write:

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

Calculating probabilities

If the Markov chain is homogeneous, we have:

$$
\begin{aligned}
& P(X_0 = i_0, X_1 = i_1, \ldots, X_{n+1} = i_{n+1}) \\
= \quad & P(X_0 = i_0) \cdot \prod_{k=0}^{n} P(X_{k+1} = i_{k+1} | X_k = i_k) \\
= \quad & P(X_0 = i_0) \cdot \prod_{k=0}^{n} p_{i_k i_{k+1}}
\end{aligned}
$$

The probabilities of the whole trajectories of the Markov Chain is determined by the transition probabilities and the initial distribution of X_0.

Transition Probability Matrix

One-step transition probability matrix

Markov Chain with state space $S = \{1, 2, \ldots, M\}$

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1M} \\ p_{21} & p_{22} & \cdots & p_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ p_{M1} & p_{M2} & \cdots & p_{MM} \end{pmatrix}$$

Properties:

- Rows add up to 1
- All entries are non-negative

Transition Probability Matrix Example

Example: Weather

Define three possible states for the weather:

1) Sunny 2) Rainy 3) Snowy

Assume that the daily weather can be described by a homogeneous Markov Chain with transition probability matrix:

$$P = \begin{pmatrix} 0.6 & 0.3 & 0.1 \\ 0.1 & 0.7 & 0.2 \\ 0.2 & 0.3 & 0.5 \end{pmatrix}$$

Two-step Transition Probabilities

Definition: The probability of moving from state i to j in two steps is

$$\mathbb{P}(X_{n+2} = j \mid X_n = i).$$

Derivation:

$$\begin{aligned}
\mathbb{P}(X_{n+2} = j \mid X_n = i) &= \sum_k \mathbb{P}(X_{n+2} = j \mid X_{n+1} = k, X_n = i)\, \mathbb{P}(X_{n+1} = k \mid X_n = i) \\
&= \sum_k \mathbb{P}(X_{n+2} = j \mid X_{n+1} = k)\, p_{ik} \\
&= \sum_k p_{kj}\, p_{ik}
\end{aligned}$$

This is entry (i, j) of matrix P^2. The two-step transition probability is P^2.

Theorem: m-step Transition Probability Matrix

If P is the one-step transition probability matrix of a homogeneous Markov chain, then the m-step transition probability matrix is P^m.

Transition Probability Matrix Example

Example: Wheather (cont.)

If today (Monday) is sunny, what is the probability that Thursday will be sunny again?

Thursday is three days from today so we compute the 3-step transition probability matrix P^3.

$$P^3 = \begin{pmatrix} 0.3220 & 0.4680 & 0.2100 \\ 0.2100 & 0.5320 & 0.2580 \\ 0.2580 & 0.4680 & 0.2740 \end{pmatrix}$$

Answer: 0.3220, which is the entry $(1, 1)$ of matrix P^3.

Transition Probability Matrix Example

Example: Wheather (cont.)

Limiting behaviour (rounded to 4 decimal places).

$$P^{10} = \begin{pmatrix} 0.2502 & 0.4999 & 0.2498 \\ 0.2498 & 0.5001 & 0.2501 \\ 0.2501 & 0.4999 & 0.2499 \end{pmatrix}$$

$$P^{20} = \begin{pmatrix} 0.2500 & 0.5000 & 0.2500 \\ 0.2500 & 0.5000 & 0.2500 \\ 0.2500 & 0.5000 & 0.2500 \end{pmatrix}$$

Observation: The effect of the initial state becomes negligible.

Distribution of the Chain

Suppose that $s \in \mathbb{R}^M$ (row vector) represents the distribution (probability mass function) of the Markov chain at time n.

The distribution of the chain at time $n+1$ will be sP

In general the distribution of the chain at time $n+m$ will be sP^m

Stationary Distribution

Definition: A distribution vector $s \in \mathbb{R}^M$ is said to be stationary for a Markov chain with one-step probability distribution P if $s = sP$.

Interpretation: If the distribution (p.m.f.) of X_0 is s, then the distribution of X_n is s for all n.

Transition Probability Matrix Example

Example: Weather (cont.)

$$\begin{pmatrix} 0.25 & 0.5 & 0.25 \end{pmatrix} \begin{pmatrix} 0.6 & 0.3 & 0.1 \\ 0.1 & 0.7 & 0.2 \\ 0.2 & 0.3 & 0.5 \end{pmatrix} = \begin{pmatrix} 0.25 & 0.5 & 0.25 \end{pmatrix}$$

This means that $s = \begin{pmatrix} 0.25 & 0.5 & 0.25 \end{pmatrix}$ is a stationary distribution for that Markov chain.

In general there may be more than one stationary distribution for a Markov Chain, but in most "interesting" cases there is only one stationary distribution.

Under certain conditions, it can be proven a connection between the stationary distribution and the limiting behaviour of a Markov chain.

Generation of Markov Chains

The following algorithm can be used to generate paths of a Markov Chain with arbitrary length n (meaning that we have to generate the sequence $X_0, X_1, \ldots, X_n$)

Algorithm 1 Generate a Markov Chain trajectory

1: Generate X_0 according to the initial distribution.
2: **for** $k = 1$ to n **do**
3: Generate $X_k \in S$ with probability

$$P(X_n = j) = p_{x_{n-1},j}$$

4: **end for**
5: **return** $(X_0, X_1, \ldots, X_n)$

Example: Simulating a Markov Chain

Consider a Markov Chain taking values in $S = \{1, 2\}$ with initial distribution

$$P(X_0 = 1) = 0.3, \quad P(X_0 = 2) = 0.7,$$

and transition matrix

$$P = \begin{bmatrix} 0.5 & 0.5 \\ 0.6 & 0.4 \end{bmatrix}$$

Generate a path of this Markov Chain with length $n = 40$.

R Code

```r
n <- 40
P <- matrix(c(0.5,0.6,0.5,0.4),2,2)
X <- vector()
U <- runif(1)
U1 <- runif(n)
if (U < 0.3) {X[1] <- 1}
else {X[1] <- 2}

for (i in c(1:n)) {
  if (U1[i] < P[X[i],1]) {
    X[i+1] <- 1
  } else {
    X[i+1] <- 2
  }
}
A <- c(0:n)
plot(A, X, type="s")
```

Python Code

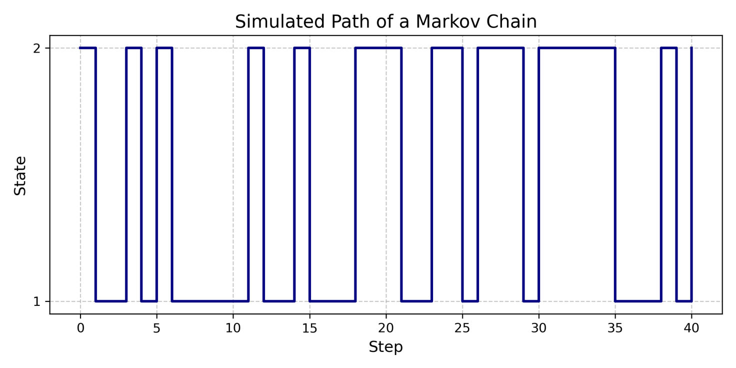
```python
import numpy as np
import matplotlib.pyplot as plt

n = 40
P = np.array([[0.5, 0.5],
              [0.6, 0.4]])
X = np.zeros(n+1, dtype=int)
U = np.random.rand()
if U < 0.3: X[0] = 1
else: X[0] = 2

U1 = np.random.rand(n)

for i in range(n):
    if U1[i] < P[X[i]-1, 0]:
        X[i+1] = 1
    else:
        X[i+1] = 2

plt.step(range(n+1), X)
plt.show()
```



Simulated trajectory of a 2-state Markov Chain with $n = 40$.

Remarks:

- The code shown before is not the most compact/efficient for the generation of Markov Chain paths.
- A more efficient approach is to use **categorical sampling**:
  - In **R**: use *`sample()`* or *`rmultinom()`*.
  - In **Python**: use *`numpy.random.choice()`* (or *`torch.multinomial()`* for GPU).
- **Complexity:** generating a single path of length n requires $O(n)$ categorical draws. The vectorized implementations are much faster when simulating many independent paths.
- Efficient Markov Chain simulation is especially important in **MCMC** (Markov Chain Monte Carlo), where one often needs to generate millions of steps or multiple chains.

Homework

Consider a Markov Chain taking values in $S = \{1, 2, 3\}$ with initial distribution $X_0 = 2$ and

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

Generate a path of this Markov Chain with length $n = 40$.