STAT5003

Week 11 : Markov Chain Monte Carlo

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Markov Chain Monte Carlo

Markov Chain Monte Carlo

- Markov Chain Monte Carlo (MCMC) is a Monte Carlo sampling technique for generating samples from an arbitrary distribution
- The difference between MCMC and Monte Carlo simulation from last week is that it uses a Markov Chain
- Two popular implementations of MCMC are
  - Metropolis-Hastings algorithm (core by Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller (1953) and generalization by Hastings (1970))
  - Gibbs samplers.

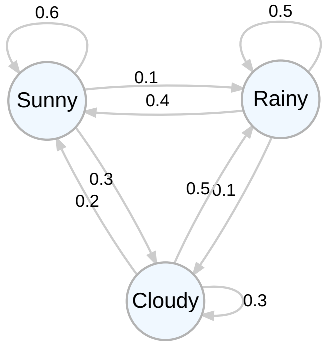
Markov Chains

What are Markov Chains?

- Markov chain is a stochastic process that follows the Markov property
- Markov property means that the future state of the process only depends on the current state
  - Consider a **dependent sequence** where each point only depends on the immediate past.
  - Sequence $\{X_1, X_2, \ldots, X_n\}$
  - Probabilities $P(X_n|X_{n-1}, X_{n-2}, \ldots, X_1) = P(X_n|X_{n-1})$
- Almost Memory-less system 几乎无内存系统

Markov state diagrams

- Represent states as the vertices of the graph
- Edges represent the probability of moving from one state to another state
  - e.g. if it is sunny today, 10% chance of being rainy tomorrow
- Can use this state diagram to construct a sequence of states

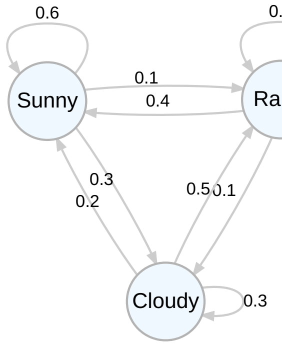


Transition Probability Matrix

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

- Rows represent current state
- Columns represent next state

$$P_{ij} = \text{probability of transititioning from state } i \text{ to state } j$$



Transition Probability Matrix

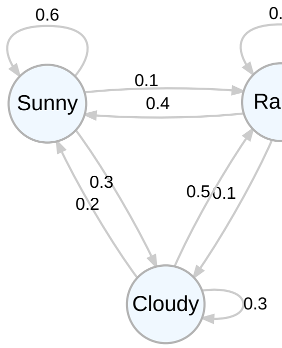
- Start with a sunny day on day 0

$$p_0 = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$$

$$p_1 = p_0 P = \begin{array}{c} \begin{matrix} s & r & c \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \end{array} \begin{pmatrix} 0.6 & 0.1 & 0.3 \\ 0.4 & 0.5 & 0.1 \\ 0.2 & 0.5 & 0.3 \end{pmatrix}$$

$$p_1 = \begin{pmatrix} 0.6 & 0.1 & 0.3 \end{pmatrix}$$
$$p_2 = \begin{pmatrix} 0.46 & 0.26 & 0.28 \end{pmatrix}$$
$$p_3 = \begin{pmatrix} 0.436 & 0.316 & 0.248 \end{pmatrix}$$
$$p_4 = \begin{pmatrix} 0.4376 & 0.3256 & 0.2368 \end{pmatrix}$$

- $\boxed{\text{Eventually converges to an invariant distribution}}$



Invariant distribution

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- For regular Markov chains, the probability vector p_t converges to the invariant distribution π in the limit
- Can also be represented as:

$$\pi = \pi P$$

- This is satisfied if the Markov chain is :

1. **Irreducible** - i.e. there is a path from every vertex to every other vertex

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2. **Aperiodic** – i.e. there are no loops in the Markov chain. If this is not satisfied, then the system will oscillate

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MCMC - Metropolis-Hasting algorithm

Metropolis-Hasting algorithm - Intuition

- Travelling politician problem
- Imagine you are a politician trying to visit all the town halls in your electorate and you want to spend time proportional to the number of voters in each town hall
- You start at a random town hall
- Choose the next town hall to visit
  - If the new town hall has more voters than your current town hall, then go there
  - If not, then go there with a probability that is equal to Number of people in new town hall / Number of people in current town hall

Metropolis-Hastings algorithm

- Similar to the acceptance-rejection method
  - it simulates a trial state
  - accepts or rejects it according to some random mechanism
- Uses the Markov chain because each trial state depends on the previous state – almost memoryless system.
- Aim is to construct a Markov chain X_t , $t = 0, 1, \ldots$ such that the limiting distribution is $f(x)$

Metropolis-Hastings algorithm

Initialise state to X_0. Require as input a target pdf $f(x)$ and a proposal pdf $q(x, y)$

For $t = 0, 1, \ldots, N-1$ do:

- Draw $Y \sim q(x|X_t)$
- Calculate acceptance probability $\alpha(X_t, Y)$
- Define $\alpha(x, y) = \min\left\{\frac{f(y)q(x|y)}{f(x)q(y|x)}, 1\right\}$
- Draw $U \sim U(0, 1)$
- if $U \leq \alpha$ then $X_{t+1} \leftarrow Y$ else $X_{t+1} \leftarrow X_t$

Return $X_1, X_2, \ldots, X_N$

Proposal function

- If the proposal density function is symmetric,
    - $q(y|x) = q(x|y)$
    - the acceptance probability has a simpler form.
    - the MCMC algorithm is also known as a **random walk sampler**.
- One common choice of a symmetric proposal function is just the Gaussian function i.e. $q(x) \sim \mathcal{N}(x_t, \sigma)$
- The choice of σ affects how quickly the state space is explored.

Applications of MCMC

Where would you use MCMC

- One common application of MCMC is to draw from the posterior distribution in Bayesian statistical methods.

$$P(A|B) = \frac{P(B|A)}{P(B)} P(A)$$

- Posterior: The likelihood of A occurring given B has occurred.
- Likelihood ratio: The support B provides for A
- Prior: The probability of A before any data is gathered.

The posterior distribution

- Can use the Bayes rule for modelling and data.

$$P(\phi|D) = \frac{P(D|\phi)}{P(D)} P(\phi)$$

- Posterior: The likelihood of ϕ occurring given the data D.
- Likelihood ratio: The support D provides for ϕ
- Prior: The probability of ϕ before any data is gathered.

- Typically $P(D)$ is a difficult integral to evaluate.

$$P(D) = \int P(D|\phi) P(\phi)\, d\phi$$

Example involving Regression

$$P(\phi|D) = \frac{P(D|\phi)}{P(D)} P(\phi)$$

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon; \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2)$$

- $\phi = \{\beta_0, \beta_1, \ldots, \beta_p, \sigma^2\}$
- $D = \{Y_1, Y_2, \ldots, Y_n, X_{11}, X_{12}, \ldots, X_{np}\}$
- $P(D|\phi)$ will be Gaussian.
- $P(D)$ is not so easy to compute.
- $P(\phi)$ what do I choose for the prior.

Estimating posterior with MCMC

- In the Metropolis-Hastings algorithm, we only need to calculate

$$\alpha = \frac{P(\phi'|D)}{P(\phi|D)} = \frac{P(D|\phi')P(\phi')}{P(D|\phi)P(\phi)}$$

- Since $P(D)$ doesn't depend on ϕ, it cancels out on the right hand side of the above formula and hence it isn't included in the formula.

Example

Observe a series of coin flips

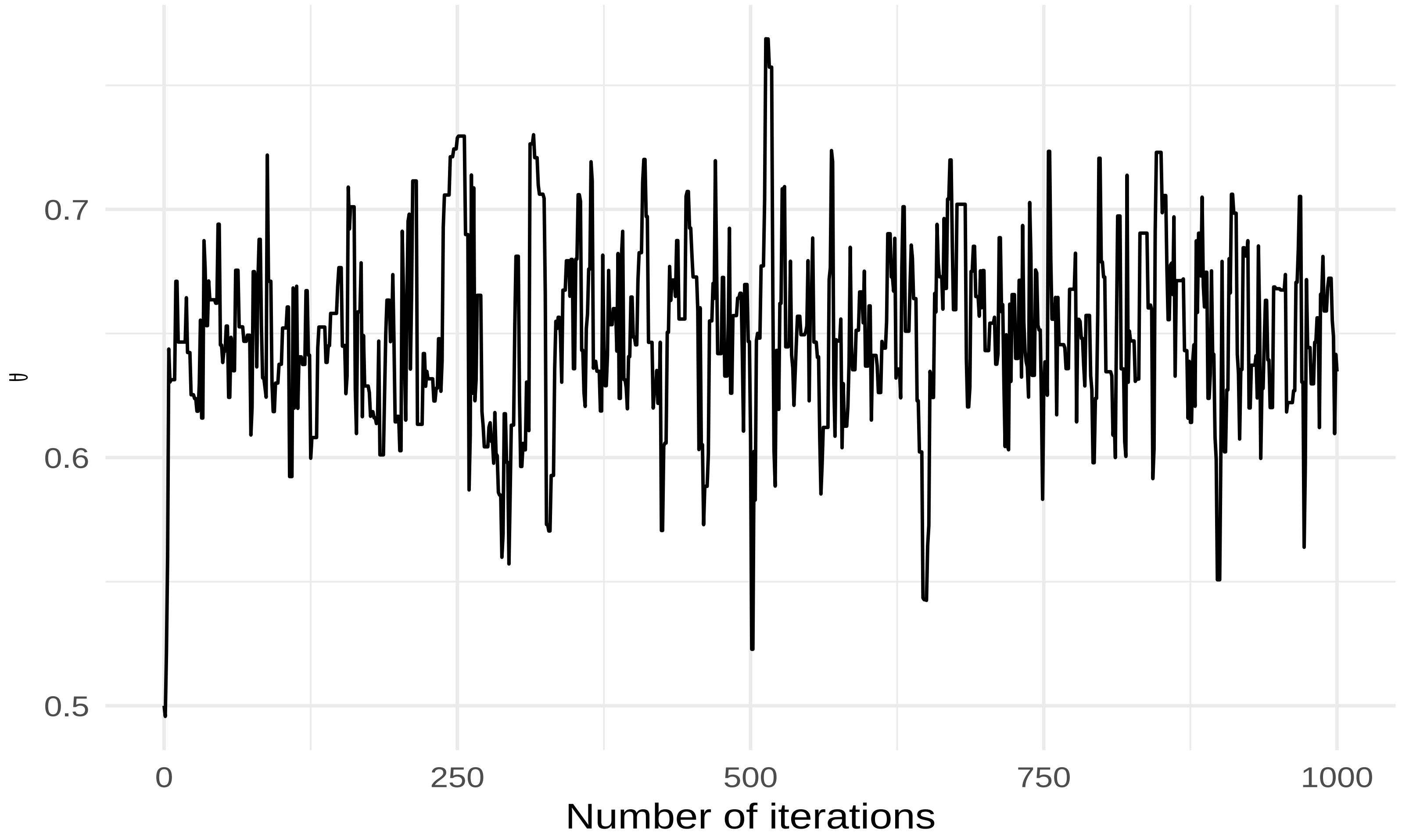
H, T, H, H, T, H, T, H, H, T, H, H, H, T, H, H, H, T, H, H, ...

Can you estimate the $P(Head)$ of this coin?

Assume you don't know anything about this coin and it could be biased!

- $\theta =$ P(Head)
- Frequentist perspective: θ is fixed but unknown
- Bayesian perspective: θ is a random variable, can compute the likelihood of θ given the observed data.
- θ_0 set as an initial point.
- Compute θ_t as a Markov chain
- Use MCMC algorithm to estimate the posterior distribution of θ.

Estimate of $P(Head)$ using MCMC



MCMC Practical considerations

- The samples at the start of the MCMC chain, before the algorithm converges to the true distribution are known as the burn-in period.
    - It should be discarded
- The samples generated by MCMC are correlated since they are from a Markov chain.
    - 支持 稀释
    - Previously, many practitioners advocated **thinning** the samples by taking say every k^{th} sample.
    - This was done for a few reasons historically
        - Reduce correlations and compute standard errors more easily
        - Less space needed to store the chain.

References

Hastings, W. K. (1970). "Monte Carlo sampling methods using Markov chains and their applications". In: *Biometrika* 57.1, pp. 97-109. ISSN: 0006-3444. DOI: 10.1093/biomet/57.1.97. eprint: https://academic.oup.com/biomet/article-pdf/57/1/97/23940249/57-1-97.pdf. URL: https://doi.org/10.1093/biomet/57.1.97.

Metropolis, N., A. W. Rosenbluth, M. N. Rosenbluth, et al. (1953). "Equation of State Calculations by Fast Computing Machines". In: *The Journal of Chemical Physics* 21.6, pp. 1087-1092. DOI: 10.1063/1.1699114. eprint: https://doi.org/10.1063/1.1699114. URL: https://doi.org/10.1063/1.1699114.

Applications Monte Carlo:

It is used to value projects that require significant amounts of funds and may have future financial implications on a company.
It can be used to simulate profits or losses in the online trading of stocks.
Simulation of the values of assets and liabilities of a pension benefit scheme.
It can also be used to value complex securities such as American or European options.

Limitations of Monte Carlo Simulations

It only provides us with statistical estimates of results, not exact figures.
It is fairly complex and can only be carried out using specially designed software that may be expensive.
The complexity of the process may cause errors leading to wrong results that can be potentially misleading.
It is a complement to analytical methods. It provides only statistical estimates, not exact results.
It does not directly provide precise insights as analytical methods do. For example, it cannot reveal cause–and–effect relationships.