Introduction to Bayesian Modeling part 1

Jingchen (Monika) Hu

Vassar College

Statistical Data Privacy

Outline

- Introduction
- 2 The foundation of Bayesian inference
- 3 Markov chain Monte Carlo: estimation and diagnostics
- Summary and References

Outline

- Introduction
- The foundation of Bayesian inference
- Markov chain Monte Carlo: estimation and diagnostics
- 4 Summary and References

Frequentist / classical and Bayesian inference

- ullet Statistical inference aims to use data $oldsymbol{Y}$ to learn about some unknown parameters $oldsymbol{ heta}$
- Frequentist / classical inference:
 - Data Y are a repeatable random sample from a statistical model or a finite population
 - Underlying parameters θ remain constant during this hypothetical repeatable process; considered fixed

Frequentist / classical and Bayesian inference

- ullet Statistical inference aims to use data $oldsymbol{Y}$ to learn about some unknown parameters $oldsymbol{ heta}$
- Frequentist / classical inference:
 - Data Y are a repeatable random sample from a statistical model or a finite population
 - Underlying parameters θ remain constant during this hypothetical repeatable process; considered fixed
- Bayesian inference:
 - ▶ Data **Y** are fixed; they are observed from the realized sample
 - Underlying parameters θ are unknown, and can be described **probabilistically**

Bayesian inference

- ullet We can use probability distributions to describe the unknown underlying parameters $oldsymbol{ heta}$
- These distributions represent our belief / knowledge about the values of the parameters
- The collected data can further sharpen / update our belief about the parameters

Outline

- Introduction
- 2 The foundation of Bayesian inference
- 3 Markov chain Monte Carlo: estimation and diagnostics
- 4 Summary and References

The setup

- We will use a toy example of a coin flipping trial to introduce the foundation
- The outcome is either a head or tail
- The data / outcome is denoted as Y
- ullet The parameter of interest is the probability of flipping a head, denoted as heta

The setup

- We will use a toy example of a coin flipping trial to introduce the foundation
- The outcome is either a head or tail
- The data / outcome is denoted as Y
- ullet The parameter of interest is the probability of flipping a head, denoted as heta
- The foundation topics include:
 - Prior
 - Likelihood
 - ▶ Bayes' rule (discrete and continuous) and posterior

- \bullet Before observing the data, we may have certain beliefs about this unknown parameter θ
- To describe our beliefs probabilistically
- Examples:
 - We know with certainty that this coin is fair: $\theta = 0.5$ with probability 1

- \bullet Before observing the data, we may have certain beliefs about this unknown parameter θ
- To describe our beliefs probabilistically
- Examples:
 - lacktriangle We know with certainty that this coin is fair: heta=0.5 with probability 1
 - An unfair coin which turns up heads 30% of the times: $\theta=0.3$ with probability 1

- \bullet Before observing the data, we may have certain beliefs about this unknown parameter θ
- To describe our beliefs probabilistically
- Examples:
 - lacktriangle We know with certainty that this coin is fair: heta=0.5 with probability 1
 - An unfair coin which turns up heads 30% of the times: $\theta = 0.3$ with probability 1
 - ▶ Really no idea and θ can be anywhere in [0, 1] with equal probability: $\theta \sim \text{Uniform}(0, 1)$

- \bullet Before observing the data, we may have certain beliefs about this unknown parameter θ
- To describe our beliefs probabilistically
- Examples:
 - lacktriangle We know with certainty that this coin is fair: heta=0.5 with probability 1
 - An unfair coin which turns up heads 30% of the times: $\theta = 0.3$ with probability 1
 - ▶ Really no idea and θ can be anywhere in [0, 1] with equal probability: $\theta \sim \text{Uniform}(0, 1)$
 - ▶ Half the times $\theta = 0.3$ and half the times $\theta = 0.7$: $\theta = 0.3$ with probability 0.5 and $\theta = 0.7$ with probability 0.5

Prior in Bayesian inference

- Bayesian inference combines our prior belief with the information contained in the collected data
- In our toy example:
 - lacktriangle Prior refers to our belief about heta before we start collecting data
 - Collecting data refers to the coin flipping trial
 - lackbox Posterior refers to out belief about heta after we collect and analyze our data

Prior in Bayesian inference

- Bayesian inference combines our prior belief with the information contained in the collected data
- In our toy example:
 - lacktriangle Prior refers to our belief about heta before we start collecting data
 - Collecting data refers to the coin flipping trial
 - lackbox Posterior refers to out belief about heta after we collect and analyze our data
- Discussion question: If we start with a fair coin prior belief, and we see an outcome of head, how would you use this collected data to update your belief? What if we see 5 heads in a row?

Expressing a prior

• Three examples of discrete prior for θ :

Value of θ	Case 1: $Pr(\theta)$	Case 2: $Pr(\theta)$	Case 3: $Pr(\theta)$
0.3	0.333	0.25	0.5
0.5	0.333	0.25	0.25
0.7	0.333	0.5	0.25

Expressing a prior

• Three examples of discrete prior for θ :

Value of θ	Case 1: $Pr(\theta)$	Case 2: $Pr(\theta)$	Case 3: $Pr(\theta)$
0.3	0.333	0.25	0.5
0.5	0.333	0.25	0.25
0.7	0.333	0.5	0.25

- Examples of continuous prior for θ :
 - $\theta \sim \mathrm{Uniform}(0,1)$ (i.e., θ can be anywhere in [0, 1] with equal probability)

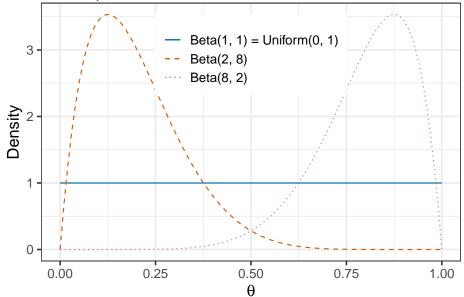
Beta prior for θ

- ullet A common choice for continuous prior for $heta \in [0,1]$
- The probability density function of Beta(a, b) is:

$$f(\theta) = \frac{\theta^{a-1}(1-\theta)^{b-1}}{B(a,b)}, \theta \in [0,1], a > 0, b > 0,$$
 (1)

where $B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$ and $\Gamma(\cdot)$ is the gamma function. The mean and variance of $\theta \sim \text{Beta}(a,b)$ are a/(a+b) and $ab/((a+b)^2(a+b+1))$ respectively.

Three beta priors



Comments on priors

- Bayesian inference is subjective
- Each person might have a different way to describe the underlying parameter θ probabilistically
- We can incorporate useful information about the unknown parameter θ , if we do have such useful information

Likelihood

- Bayesian inference combines our prior belief with the information contained in the collected data
- The collected data can be expressed as a model describing the distribution of the data as a function of the parameters
- We will refer to this data model as likelihood: a probability distribution of the data as a function of the parameters

Review: the Bernoulli distribution

The probability mass function of $Bernoulli(\theta)$ is:

$$f(Y = y \mid \theta) = \theta^{y} (1 - \theta)^{1 - y}, y = \{0, 1\}, \theta \in [0, 1].$$
 (2)

The mean and variance of $Y \sim \operatorname{Bernoulli}(\theta)$ is θ and $\theta(1-\theta)$ respectively.

Bernoulli likelihood for Y

From this Bernoulli probability mass function, we can write our likelihood function as:

$$L(\theta) = \theta^{y} (1 - \theta)^{1 - y}. \tag{3}$$

- The likelihood is a function of θ (recall in Bayesian inference, data are considered fixed and parameters are considered random)
- Bayes' rule will help us to combine prior and data to posterior

Discrete Bayes' rule and posterior

• If we start with $\theta = \{0.3, 0.5, 0.7\}$ with equally probability of 0.333... for each, after seeing a flipped head, what are our updated probability of each of the possible values?

Discrete Bayes' rule and posterior

- If we start with $\theta = \{0.3, 0.5, 0.7\}$ with equally probability of 0.333... for each, after seeing a flipped head, what are our updated probability of each of the possible values?
- The discrete Bayes' rule:

$$\pi(\theta = \theta_c \mid y) = \frac{f(y \mid \theta_c)\pi(\theta_c)}{\sum_j f(y \mid \theta_j)\pi(\theta_j)} = \frac{L(\theta_c)\pi(\theta_c)}{\sum_j L(\theta_j)\pi(\theta_j)},\tag{4}$$

- ► The denominator is the marginal probability of y by the Law of Total Probability, i.e. $\sum_i L(\theta_i)\pi(\theta_i) = \sum_i f(y \mid \theta_i)\pi(\theta_i) = f(y)$
- ▶ $L(\theta_c)$ is our likelihood function of observing y given θ_c
- Discussion question: Calculate the posterior probability of $\theta = 0.3$ after seeing one head (i.e., y = 1).

Use R for posterior calculation

```
theta <-c(0.3, 0.5, 0.7)
y <- 1
likelihood <- stats::dbinom(x = y, size = 1, prob = theta)
likelihood
## [1] 0.3 0.5 0.7
prior \leftarrow c(1/3, 1/3, 1/3)
product <- prior * likelihood</pre>
product
## [1] 0.1000000 0.1666667 0.2333333
product / sum(product)
```

[1] 0.2000000 0.3333333 0.4666667

The posterior

Value				
of θ	$\pi(heta)$	$f(y \mid \theta)$	$f(y \mid \theta)\pi(\theta)$	$\pi(\theta \mid y)$
0.3	0.333	0.3	0.100	0.200
0.5	0.333	0.5	0.167	0.333
0.7	0.333	0.7	0.233	0.467

Continuous Bayes' rule and posterior

- If we start with a beta prior distribution for θ , what is our posterior distribution for θ after seeing a flipped head?
- The continuous Bayes' rule:

$$\pi(\theta \mid y) = \frac{f(y \mid \theta)\pi(\theta)}{\int_{\theta'} f(y \mid \theta')\pi(\theta')d\theta'} = \frac{L(\theta)\pi(\theta)}{\int_{\theta'} L(\theta')\pi(\theta')d\theta'}.$$
 (5)

► The denominator is the marginal probability of f(y), i.e. $\int_{\theta'} L(\theta')\pi(\theta')d\theta' = \int_{\theta'} f(y \mid \theta')\pi(\theta')d\theta' = \int_{\theta'} f(y,\theta')d\theta' = f(y)$, which is a constant since the data is fixed

Continuous Bayes' rule and posterior

- If we start with a beta prior distribution for θ , what is our posterior distribution for θ after seeing a flipped head?
- The continuous Bayes' rule:

$$\pi(\theta \mid y) = \frac{f(y \mid \theta)\pi(\theta)}{\int_{\theta'} f(y \mid \theta')\pi(\theta')d\theta'} = \frac{L(\theta)\pi(\theta)}{\int_{\theta'} L(\theta')\pi(\theta')d\theta'}.$$
 (5)

- ► The denominator is the marginal probability of f(y), i.e. $\int_{\theta'} L(\theta')\pi(\theta')d\theta' = \int_{\theta'} f(y \mid \theta')\pi(\theta')d\theta' = \int_{\theta'} f(y,\theta')d\theta' = f(y)$, which is a constant since the data is fixed
- Typically we use this following version of the continuous Bayes' rule:

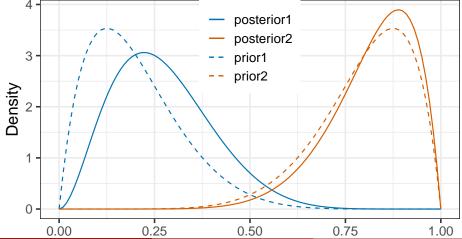
$$\pi(\theta \mid y) \propto f(y \mid \theta)\pi(\theta) = L(\theta)\pi(\theta).$$
 (6)

The beta-binomial conjugacy

For a binomial data model where $Y \sim \operatorname{Binomial}(n, p)$ and p is the model parameter (the success probability), a $\operatorname{Beta}(a, b)$ prior for p gives a $\operatorname{Beta}(a + y, b + n - y)$ posterior.

Two beta priors and two beta posteriors

- Data: y = 1 (i.e., one trial and the outcome is a head)
- Prior 1: $\theta \sim \text{Beta}(2,8)$; Posterior 1: $\theta \sim \text{Beta}(3,8)$
- Prior 2: $\theta \sim \text{Beta}(8,2)$; Posterior 2: $\theta \sim \text{Beta}(9,2)$



Recap: 3 general steps in Bayesian inference

- **9 Prior** $\pi(\theta)$: Specify distributions for the parameters prior to seeing the data.
- **Q Likelihood** $L(\theta) = f(y \mid \theta)$: Choose an appropriate data model for the data generation process and create the likelihood function expression.
- **Output** Posterior $\pi(\theta \mid y)$: Use Bayes' rule to combine the prior and the data, and obtain the posterior distributions for the parameters.

Outline

- Introduction
- The foundation of Bayesian inference
- 3 Markov chain Monte Carlo: estimation and diagnostics
- 4 Summary and References

MCMC overview

- Simple Bayesian models have analytical solution to the posterior (e.g., beta-binomial conjugacy)
- More sophisticated Bayesian models (e.g., more than one parameter) require more complicated posterior estimation methods
- The general class of posterior estimation methods is called Markov chain Monte Carlo (MCMC)

MCMC estimation

- General strategy: design a Markov chain whose stationary distribution is the posterior distribution of interest
 - We set up a stochastic process which moves randomly in the space of parameters of our Bayesian model such that after a certain time, the process will produce samples from the posterior distribution of interest
 - At each iteration, the move of the process only depends on the value of the process at the previous iteration; therefore it is a Markov chain

(more details available at Chapter 9 of Albert and Hu (2019): https://bayesball.github.io/BOOK/proportion.html)

Gibbs sampler

- To obtain a draw from a multivariate posterior distribution
- The Gibbs sampler works by simply repeatedly sampling from the posterior distribution of each parameter, conditional on the remaining parameters (i.e., the full conditional posterior distribution)

Gibbs sampler example

- ullet A normal data model with mean μ and standard deviation σ unknown
- conditional posterior distributions: $f(\mu \mid \sigma, Y)$ and $f(\sigma \mid \mu, Y)$

• Start with an appropriate prior $\pi(\mu, \sigma)$, we derive the two full

- ullet Iteratively sample draws of μ and σ in the following: at iteration s+1
 - **1** Sample $\mu^{s+1} \sim f(\mu \mid \sigma^s, Y)$.
 - 2 Sample $\sigma^{s+1} \sim f(\sigma \mid \mu^{s+1}, Y)$.

Gibbs sampler example cont'd

- After a certain number S of iterative sampling is done, we can evaluate whether the chain has converged
- If so, the collective sampled draws of $\{\mu^1, \cdots, \mu^S\}$ are an approximation to the posterior distribution of μ , and those of $\{\sigma^1, \cdots, \sigma^S\}$ are an approximation to the posterior distribution of σ

Gibbs sampler example cont'd

- After a certain number S of iterative sampling is done, we can evaluate whether the chain has converged
- If so, the collective sampled draws of $\{\mu^1,\cdots,\mu^S\}$ are an approximation to the posterior distribution of μ , and those of $\{\sigma^1,\cdots,\sigma^S\}$ are an approximation to the posterior distribution of σ
- Any posterior inferences on μ and σ can then be obtained by summarizing these posterior draws

Metropolis algorithm

 The Metropolis algorithm relies on making a proposal draw for the values of the parameters in the model, and evaluating whether we move to the proposal draw or stay at the current draw

Metropolis algorithm example

- ullet A normal data model with mean μ and standard deviation σ unknown
- We illustrate the process for μ (updating of σ follows a similar approach)
- A Metropolis algorithm has three general steps at iteration s + 1:
 - ① Given the current simulated value μ^s , we propose a new value μ^* , selected at random from a uniform with width 2C (i.e. from the interval of $(\mu^s C, \mu^s + C)$ or other symmetric distributions (e.g. normal centered at μ^s).
 - ② Compute the ratio R of the posterior density (denoted as $\pi_n(\mu)$) at the proposed value μ^* and at the current value μ^s : $R = \pi_n(\mu^*)/\pi_n(\mu^s)$; from this we obtain an acceptance probability of $p = \min\{R, 1\}$.
 - § Simulate a uniform random variable from [0, 1], denoted as U. If U < p, we move to the proposed value μ^* , and otherwise we stay at the current value μ^s .

Hamiltonian Monte Carlo and Stan

- Not all models are amenable to Gibbs sampler or Metropolis
 algorithm, and in some cases these algorithms can take a long time to
 converge due to their random walk nature
- The Hamiltonian Monte Carlo (HMC) sampling algorithm is one of the more recent posterior sampling algorithms that is gaining popularity

Hamiltonian Monte Carlo and Stan

- Not all models are amenable to Gibbs sampler or Metropolis algorithm, and in some cases these algorithms can take a long time to converge due to their random walk nature
- The Hamiltonian Monte Carlo (HMC) sampling algorithm is one of the more recent posterior sampling algorithms that is gaining popularity
- In this course, we use the brms R package to estimate Bayesian models for statistical data privacy purposes, most often for generating synthetic data
- The brms package relies on HMC
- The estimation output will return the complete sequence of draws for each of the parameters in the model

MCMC diagnostics for convergence

- The obtained posterior draws from MCMC estimation can be used for posterior inference only once we can confirm that they serve as a good approximation to the true posterior distribution (i.e., enough iterations have occurred for the MCMC to have converged to the true posterior)
- While no test can guarantee that the MCMC has indeed converged to its stationary distribution, we can use several diagnostic tools to identify obvious issues showing that the MCMC has not converged

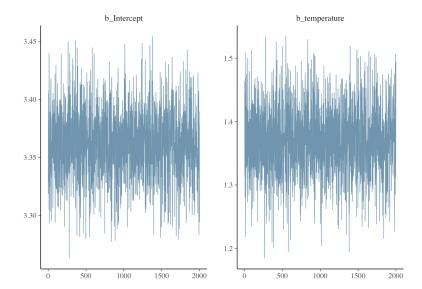
Traceplots and autocorrelation plots

have extensively explored the parameter space and are relatively independent from each other

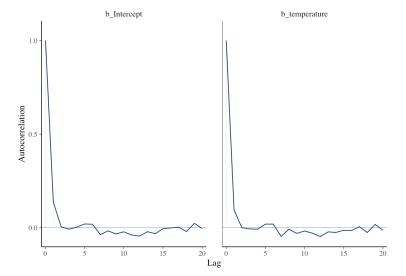
A converged MCMC should include posterior parameter draws that

- We can check by using traceplots: plot the parameter values against each MCMC iteration number
- We can also check by using autoccorelation plots to see if the posterior draws are relatively independent from each other

Traceplots example



Autocorrelation plots example



Burn-in, thinning, and multiple MCMC chains

- Suppose the MCMC has been run for S iterations
- **Burn-in**: After iteration S^* (at which point we believe the chain has converged), we discard all draws before this iteration; this period is called the burn-in period; inference will only be using the remaining $S-S^*$ draws

Burn-in, thinning, and multiple MCMC chains

- Suppose the MCMC has been run for S iterations
- **Burn-in**: After iteration S^* (at which point we believe the chain has converged), we discard all draws before this iteration; this period is called the burn-in period; inference will only be using the remaining $S-S^*$ draws
- **Thinning**: To get rid of the autocorrelation between the draws, we can keep one of every k-th sample, e.g., k=10; this procedure is called thinning; inference will only be using the remaining $(S-S^*)/k$ draws

Burn-in, thinning, and multiple MCMC chains

- Suppose the MCMC has been run for S iterations
- **Burn-in**: After iteration S^* (at which point we believe the chain has converged), we discard all draws before this iteration; this period is called the burn-in period; inference will only be using the remaining $S-S^*$ draws
- **Thinning**: To get rid of the autocorrelation between the draws, we can keep one of every k—th sample, e.g., k=10; this procedure is called thinning; inference will only be using the remaining $(S-S^*)/k$ draws
- Run multiple chains at different starting points to see if they arrive at a similar sample space

A brms example

- We will learn this example in the next lecture
- Discussion question: Identify S, S^* , k and the number of MCMC chains.

Outline

- Introduction
- The foundation of Bayesian inference
- 3 Markov chain Monte Carlo: estimation and diagnostics
- Summary and References

Summary

- The foundation of Bayesian inference
 - Prior
 - Likelihood
 - Bayes' rule (discrete and continuous) and posterior

Summary

- The foundation of Bayesian inference
 - Prior
 - Likelihood
 - Bayes' rule (discrete and continuous) and posterior
- Markov chain Monte Carlo (MCMC)
 - Estimation
 - Diagnostics

Summary

- The foundation of Bayesian inference
 - Prior
 - Likelihood
 - Bayes' rule (discrete and continuous) and posterior
- Markov chain Monte Carlo (MCMC)
 - Estimation
 - Diagnostics
- Homework 2: a few derivation and R programming exercises
 - Submission on Moodle and prepare to discuss next time
- Lecture 3: Introduction to Bayesian modeling part 2
 - ► Chapter 11 of Albert and Hu (2019): https://bayesball.github.io/BOOK/proportion.html (a different MCMC software is used)

References I

Albert, J., and J. Hu. 2019. <u>Probability and Bayesian Modeling</u>. Texts in Statistical Science, Chapman Hall CRC Press.