

Mathematical Statistics II

The Bayesian Approach to Parameter Estimation

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Introduction

Bayesian Estimation

- Much of this work is based on Rice (2007, Section 8.6).
- We have already discussed the philosophy of Bayesian statistics. HB, EB, Jeffrey's Priors, Integration.
- We start with a prior belief about parameter values, and update these beliefs using observed data.
- The resulting **distribution** is called the *posterior*, and it represents our updated belief after observing data.
- This is very natural idea that is closely related to the idea of likelihood: likelihood quantifies some degree of belief about a parameter value.

Review

Some Review

- Before we begin, we will first do a bit of review.
- In the context of Bayesian inference, we treat unknown parameter vectors as random variables, which I will denote Θ .
- Thus, our probability model can be expressed as $f(x|\underline{\Theta} = \theta)$, which we often shorten to $f(x|\theta)$.

$$\begin{array}{c} \underline{f(x|\theta)} \\ \uparrow \\ \underline{f(x|\theta = \theta)} \end{array}$$

$$\begin{array}{c} \boxed{\underline{f(x|\theta)}} \leftarrow \\ \uparrow \\ \text{John Rice} \\ \text{text.} \end{array}$$

Some Review II

Bayes' Theorem

Let X be the random vector representing observed data, and Θ the random parameter vector, and x^* the observed data. Bayes Theorem states:

$$\begin{aligned}\pi_{\Theta|X}(\theta|x^*) &= \frac{f_{X|\Theta}(x^*|\theta)\pi_{\Theta}(\theta)}{f_X(x^*)} \\ &= \frac{f_{X|\theta}(x^*|\theta)\pi_{\Theta}(\theta)}{\int f_{X|\Theta}(x^*|\tau)\pi_{\Theta}(\tau) d\tau}\end{aligned}$$

- As before, f is taken to be either a pmf or pdf, depending on the problem.

Some Review III

Flipping 10 coins

Our friend hands us a coin from another country, and we want to estimate $\theta = p$, the probability that the coin lands heads.

Suppose we flip a coin 10 times, and see n heads. Find a Bayesian estimate for θ .

$$X = \# \text{ heads,}$$

$$X = x^* = n$$

$$X|\theta = \theta \sim \text{Bin}(10, p = \theta)$$

$$\frac{f_{X|\theta}(x^*|\theta)}{f_{X|\theta}(x^*|\theta)} = \frac{\binom{10}{n} \theta^n (1-\theta)^{10-n}}{\binom{10}{n} \theta^n (1-\theta)^{10-n}}$$

- "I know nothing about the coin, so all prob. are equally likely" $\Theta \sim U(0,1)$

$$\rightarrow \pi_{\Theta}(\theta) = \mathbb{I}(0 \leq \theta \leq 1)$$

$$\star \pi_{\Theta|X=n}(\theta|x^*) = \frac{f_{X|\Theta}(x^*|\theta) \pi_{\Theta}(\theta)}{\int f_{X|\Theta}(x^*|\gamma) \pi_{\Theta}(\gamma) d\gamma}$$

$$\star \pi(\theta | x^*) = \frac{f(x^* | \theta) \pi(\theta)}{\int f(x^* | z) \pi(z) dz} \quad \left. \begin{array}{l} \text{move} \\ \text{common} \end{array} \right\}$$

$$\pi(\theta | x^*) = \frac{\binom{10}{n} \theta^n (1-\theta)^{10-n}}{\int_0^1 \binom{10}{n} z^n (1-z)^{10-n} dz} \mathbb{I}[0 \leq \theta \leq 1]$$

↑
Beta dist'n integral

$$= \frac{\Gamma(10+1)}{\Gamma(n+1)\Gamma(10-n+1)} \theta^n (1-\theta)^{10-n} \mathbb{I}[0 \leq \theta \leq 1]$$

$$\Theta | X=x^*=n \sim \text{Beta}(n+1, 10-n+1)$$

$$\underline{\underline{E[\Theta | x^*] = \frac{n+1}{10+2}}}$$

$$\left(\text{MLE: } \hat{\Theta}_{\text{MLE}} = \frac{n}{10} \right)$$

$$\hat{\Theta}_{\text{MLE}} = \frac{6}{10} \approx 0.6$$

$$\rightarrow E[\Theta | x^*] = \frac{7}{12} \approx \underline{\underline{0.58}}$$

• posterior Mode :



Mode of Beta(α, β):

$$\frac{\alpha - 1}{\alpha + \beta - 2}$$

$$\hat{\theta}_{MLE}$$

||

so for our example:

$$\text{mode} = \frac{(n+1) - 1}{(n+1) + (10 - n + 1) - 2}$$

$$= \frac{n}{10}$$

$$\pi(\theta|x^*) = f(\theta, x^*)$$

$$\text{mode} = \underset{\theta}{\text{arg max}} f(\theta, x^*)$$

★ Maximum A posteriori
(MAP) estimate.

• max of posterior

= mode of posterior.

→ Median of posterior.

• Beta - no closed form solution.

f beta (0.5, α , β)

Some Review IV

- Even in the simple problem above, we see two of the primary challenges with Bayesian parameter estimation:
 - How do we choose the prior distribution $\pi(\theta)$? A generally safe and accepted approach is a uniform prior. However, this formally only exists if θ is bounded, which is not always the case. Also, it represents a prior belief: given a new coin, do we really think all values of p are equally likely, or maybe values close to $p = 0.5$ are more likely than extreme values $p = 0, 1$? Since the prior represents our beliefs about θ , is a uniform prior actually appropriate? If it isn't appropriate, how exactly should we specify the prior?
 - Even in this very simple model and prior, the denominator $f(x)$ was difficult to compute. What about more complex models and priors? A large amount of Bayesian computation and theory is dedicated to solving this problem.

$$\underline{\pi(\theta|x)} = \frac{L(\theta)\pi(\theta)}{\int L(\gamma)\pi(\gamma)d\gamma}$$

$$\int \pi(\theta|x) d\theta = 1$$

$$\pi(\theta|x) \propto L(\theta)\pi(\theta)$$

conjugate priors :-

Some Review V

Proposition: the MAP and MLE

Let θ be a parameter of interest, and x^* the observed data. If our prior distribution is proportional to 1, i.e., $\pi(\theta) \propto 1$ (which is effectively a uniform prior on a bounded interval), then

$$\hat{\theta}_{\text{MAP}} = \hat{\theta}_{\text{MLE}}.$$

- This is true for the Coin-tossing example; look back at the likelihood function and posterior, and use R to plot them both.

posterior mean: $E[\theta|x]$

MAP (mode): $\max_{\theta} \pi(\theta|x)$

median : $\text{Med}[\theta|x]$

proof sketch:

$$\pi(\theta|x) \propto L(\theta) \pi(\theta)$$

$$\text{if } \pi(\theta) \propto 1 \Rightarrow$$

$$\pi(\theta|x) \propto L(\theta) \Rightarrow$$

$$\operatorname{argmax}_{\theta} \pi(\theta|x) = \operatorname{argmax}_{\theta} L(\theta) = \hat{\theta}_{\text{MLE}}$$

~~$\hat{\theta}_{\text{MLE}} \approx \text{MAP}$~~ $\rightarrow \mathbb{E}[\theta|x]$ is preferred.

Examples

Bayesian point-estimate examples

Poisson model

Suppose we have observations n observations, which we wish to model as IID $\text{Poisson}(\lambda)$. Find a Bayesian estimate of $\Lambda = \lambda$ given the observed data x^* .

- $x_i | \Lambda = \lambda \sim \text{pois}(\lambda)$
 $f_{x_i | \Lambda}(x_i | \lambda) = \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}, \quad x_i \in \{0, 1, \dots\}$

- $f_{X | \Lambda}(x | \lambda) = \prod_{i=1}^n \left(\frac{\lambda^{x_i} e^{-\lambda}}{x_i!} \right)$

$$= \frac{\lambda^{\sum x_i} e^{-n\lambda}}{\prod_{i=1}^n x_i!}$$

posterior $\Delta | X = x^*$

$$f_{\Delta | X}(\lambda | x^*) = \frac{\lambda^{\sum x_i^*} e^{-n\lambda} \cdot f_{\Delta}(\lambda)}{\int \lambda^{\sum x_i^*} e^{-n\lambda} f_{\Delta}(\lambda) d\lambda}$$

(1) determine prior for Δ

(2) calculate the integral.

• Traditional / orthodox approach

• Pick prior first.

• $E[A] = 15$,
 ~~$Var(A) = 25$~~ } ★

• $A \sim \text{Gamma}(\alpha, \beta)$

$$E[A] = \frac{\alpha}{\beta}, \quad Var(A) = \frac{\alpha}{\beta^2}$$

$$15 = \frac{\alpha}{\beta} \quad 25 = \frac{\alpha}{\beta^2}$$

$$\dots \quad \alpha = 9, \quad \beta = 3/5$$

$$f_{\Lambda}(x) = \frac{\beta^{\alpha}}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda}, \quad \lambda > 0.$$

(Recall) :

$$f_{\Lambda|x}(\lambda/x^*) = \frac{\lambda^{\sum x_i^*} e^{-n\lambda} \cdot f_{\Lambda}(\lambda)}{\int \lambda^{\sum x_i^*} e^{-n\lambda} f_{\Lambda}(\lambda) d\lambda}$$

$$f_{\lambda|X}(\lambda|x^*) = \frac{\lambda^{\sum x_i^*} e^{-n\lambda} \cdot \lambda^{\alpha-1} e^{-\beta\lambda}}{\int_0^{\infty} \lambda^{\sum x_i^*} e^{-n\lambda} \lambda^{\alpha-1} e^{-\beta\lambda} d\lambda} \quad \mathbb{I}(\lambda > 0)$$

$$= \frac{\lambda^{\sum x_i^* + \alpha - 1} e^{-\lambda(n+\beta)}}{\int_0^{\infty} \lambda^{\sum x_i^* + \alpha - 1} e^{-\lambda(n+\beta)} d\lambda} \quad \mathbb{I}(\lambda > 0)$$

$$\propto \lambda^{\sum x_i^* + \alpha - 1} e^{-\lambda(n+\beta)} \quad \mathbb{I}(\lambda > 0)$$

$$\alpha \quad \lambda \quad \text{something} \quad e^{-\text{something}(\lambda)} \quad \underline{\underline{I(x>0)}}$$

$$X \sim \text{Gamma}(a, b)$$

$$\underline{\underline{f(x)}} \propto x^{a-1} e^{-bx} \quad I(x > 0)$$

$$a-1 = \sum x_i^* + d - 1 \quad \vdots \quad b = n + \mathbb{P}$$

$$a = \sum x_i^* + d \quad \vdots$$

$$\begin{aligned} \Delta | X = x^* &\sim \text{Gamma}(a, b) \\ &\sim \text{Gamma}\left(\sum_{i=1}^n x_i^* + \alpha, n + \beta\right) \end{aligned}$$

$$\alpha = 9, \beta = \frac{3}{5},$$

$$\Delta | X = x^* \sim \text{Gamma}\left(\sum_{i=1}^n x_i^* + 9, n + \frac{3}{5}\right)$$

Real-data example: Poisson Distribution

- Now let's look at a real-data example. These data are the 23 observations from the asbestos-filter problem.

set.seed(12345)

```
x <- c(
  31, 29, 19, 18, 31, 28, 34, 27, 34, 30, 16, 18,
  26, 27, 27, 18, 24, 22, 28, 24, 21, 17, 24
)
```

```
[1] 31 29 19 18 31 28 34 27 34 30 16 18 26 27 27 18 24 22
[19] 28 24 21 17 24
```

Real-data example: Poisson Distribution II

Comparing Estimates

Using the data above, compare estimates using the MoM, MLE, and the Bayesian approach with a Gamma prior. Also, discuss the corresponding errors related to these estimates.

Conjugate Priors

Conjugate priors

- The first approach to the Poisson(λ) example was the traditional (subjective) Bayesian, who takes seriously the choice of prior, and chose a Gamma density to aid computations.
- This approach was aided by the choice of a Gamma prior, which helped the calculation.
- This type of prior is known as a conjugate prior.

$$\underline{\pi(\theta|x)} \propto \underline{f(\theta)} \rightarrow \underline{\text{known.}}$$

Conjugate priors II

Definition: Conjugate priors

Suppose the prior distribution belongs to a family of distributions, G , and the data come from a family of distributions H .

G is said to be conjugate to H if the posterior is in the family G .

- Example: If the data-model is $\text{Poisson}(\lambda)$, then the family H is the family of Poisson distributions. The Gamma family (G) of distributions is conjugate to the Poisson family, because if Gamma is selected as the prior distribution, then the posterior distribution (under data model H) is still Gamma (G), with updated parameters.

Conjugate priors III

- Much of the Bayesian statistics of the 20th century relied on conjugate priors to help with integration, or were confined to models with very few parameters.
- Recent developments in computing, both hardware, software, and theory of Bayesian computing, has enabled fitting much more complex models using arbitrary priors.
- Still, it's worth discussing conjugate priors, and we will provide a few examples.

Conjugate priors IV

Conjugate Normals

Model $X_1, \dots, X_n \sim N(\mu, \sigma^2)$. Treating σ^2 as fixed, consider the prior for $\mu \sim N(\mu_0, \sigma_0^2)$. Find the posterior of $\mu | X = x^*$.

$$f(x^* | \mu, \sigma^2) = \prod_{i=1}^n \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2\sigma^2}(x_i^* - \mu)^2}$$

$$= \sigma^{-n} (2\pi)^{-n/2} \exp\left\{-\frac{1}{2\sigma^2} \sum (x_i^* - \mu)^2\right\}$$

$$\mu \sim N(\mu_0, \sigma_0^2)$$

$$\pi(\mu) = \frac{1}{\sigma_0 \sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma_0^2} (\mu - \mu_0)^2\right\}$$

$$\pi(\underline{\mu} | x^*) \propto \sigma^{-n} (2\pi)^{-n/2} \exp\left\{-\frac{1}{2\sigma^2} \sum (x_i^* - \mu)^2\right\} \\ \cdot \frac{1}{\sigma_0 \sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma_0^2} (\mu - \mu_0)^2\right\}$$

$$\propto \frac{\exp\left\{-\frac{1}{2\sigma^2} \sum (x_i^* - \mu)^2\right\} \exp\left\{-\frac{1}{2\sigma_0^2} (\mu - \mu_0)^2\right\}}{\quad}$$

$$= \frac{\exp\left\{-\frac{1}{2\sigma^2} \sum (x_i^* - \mu)^2 - \frac{1}{2\sigma_0^2} (\mu - \mu_0)^2\right\}}{\quad}$$

$$= \exp\left\{-\frac{1}{2\sigma^2} \left[\sum x_i^2 - 2n\mu\bar{x} + n\mu^2 \right] - \frac{1}{2\sigma_0^2} (\mu^2 - 2\mu\mu_0 + \mu_0^2) \right\}$$

$$\pi(\mu|x) \propto \exp\left\{\frac{-1}{2\sigma^2} \left[-2n\bar{x} + n\mu \right] - \frac{1}{2\sigma_0^2} \left[\mu^2 - 2\mu_0\mu \right] \right\}$$

$$\frac{-1}{2\sigma^2} n\mu^2 - \frac{1}{2\sigma_0^2} \mu^2 = \mu^2 \left(-\frac{1}{2\sigma^2} - \frac{n}{2\sigma^2\sigma_0^2} \right)$$

$$= -\frac{1}{2} \mu^2 \left(\frac{n\sigma_0^2 + \sigma^2}{\sigma^2\sigma_0^2} \right)$$

↓
a

$$= \underline{-\frac{1}{2} a \mu^2} -$$

$$\begin{aligned}
\frac{2n\mu\bar{x}}{2\sigma^2} + \frac{2\mu_0\mu}{2\sigma_0^2} &= \frac{n\bar{x}}{\sigma^2}\mu + \frac{\mu_0}{\sigma_0^2}\mu \\
&= \left(\frac{n\bar{x}}{\sigma^2} + \frac{\mu_0}{\sigma_0^2}\right)\mu \\
&= \left(\frac{n\bar{x}\sigma_0 + \mu_0\sigma^-}{\sigma_0^2\sigma^2}\right)\mu \\
&= b\mu = -\frac{1}{2}(2b\mu)
\end{aligned}$$

$$\pi(\mu|x) \propto \exp\left\{-\frac{a}{2}\left(\mu - \frac{b}{a}\right)^2\right\}$$

Completing the square:

in exponential:

$$-\frac{1}{2}(au^2 - 2bu)$$

$$= -\frac{a}{2}\left(u^2 - \frac{2b}{a}u\right)$$

$$= -\frac{a}{2}\left(u^2 - \frac{2b}{a}u + \frac{b^2}{a^2}\right) +$$

$$= -\frac{a}{2}\left(u - \frac{b}{a}\right)^2 + \text{Something}$$

Something

↓

$$\left(\frac{b^2}{a^2} \frac{a}{2}\right)$$

↑

no u

$$\pi(\mu|x) \propto \exp\left\{-\frac{a}{2}\left(\mu - \frac{b}{a}\right)^2\right\}$$

$$z \sim N(\mu_z, \sigma_z^2),$$

$$f(z) \propto \exp\left\{-\frac{1}{2\sigma_z^2}(z - \mu_z)^2\right\}$$

$$\frac{a}{2} = \frac{1}{2\sigma_z^2}$$



posterior variance

$$\frac{1}{a}$$

$$= \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}$$

Posterior mean: $\mu_z = \frac{b}{a}$

$$= \frac{n\bar{x}\sigma_0^2 + \mu_0\sigma^2}{n\sigma_0^2 + \sigma^2}$$

$\mu \sim N(\mu_0, \sigma_0^2), X_i | \mu \sim N(\mu, \sigma^2)$

$$\mu | X \sim N\left(\frac{n\bar{x}\sigma_0^2 + \mu_0\sigma^2}{n\sigma_0^2 + \sigma^2}, \frac{\sigma^2\sigma_0^2}{n\sigma_0^2 + \sigma^2}\right)$$

Conjugate priors V

Beta-Binomial conjugate relation

One example that we have actually seen already is the Beta-Binomial distributions.

The $\text{Beta}(\alpha, \beta)$ distribution is conjugate to $\text{Binomial}(n, p)$. In the coin flipping example, we selected a $\text{Beta}(1, 1)$ prior.

- This example will be a HW problem.

Posteriors and Likelihood

- In the Poisson-Gamma model, we saw that we get very similar estimates using MLE or Bayesian approaches, regardless of which prior we picked.
- We can argue why this will often be the case, especially for IID data.
- Previously, we saw:

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

- When n gets large, the likelihood dominates in this equation.
In the IID case:

$$\text{likelihood} = \prod_{i=1}^n f(x_i^* | \theta).$$

Posteriors and Likelihood II

- In particular, each new data point scales the likelihood larger and larger, to the point where the prior has little impact on the posterior distribution.
- See the accompanying Lecture 4 R code for a visual demonstration of this using the Poisson distribution.

Uniform priors

- The choice of conjugate priors is useful if we want to actually use a prior and a conjugate is available.
- A common alternative choice is a uniform prior.
- This is saying: we don't have any prior knowledge or belief about a parameter. $\frac{1}{b-a}$, $b=\infty$, $a=0$, $f(\lambda)=0$
- A uniform prior is not always possible (e.g., $\lambda > 0$ has no uniform prior), but we can approximate it.

Poisson posterior, uniform prior

Revisit the $\text{Poisson}(\lambda)$ model, while taking the alternative approach of using a uniform prior.

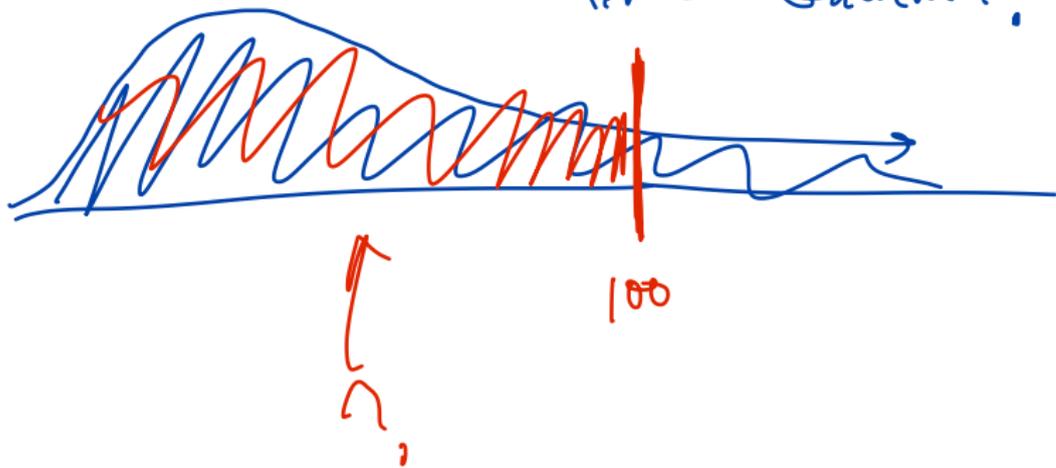
$$f(x^* | \lambda) = \prod_{i=1}^n \lambda^{x_i^*} e^{-\lambda} / C = \lambda^{\sum x_i^*} e^{-n\lambda} \cdot c^n$$

$$\pi(\lambda) = \frac{1}{100} \mathbb{I}(0 < \lambda < 100)$$

$$f_{\lambda | x^*}(\lambda | x^*) = \frac{\lambda^{\sum x_i^*} e^{-n\lambda} \cdot \frac{1}{100}}{\int_0^{100} \lambda^{\sum x_i^*} e^{-n\lambda} d\lambda} \cdot \mathbb{I}(0 \leq \lambda \leq 100)$$

$$= \frac{\lambda^{\sum x_i^*} e^{-n\lambda}}{\int_0^{100} \lambda^{\sum x_i^*} e^{-n\lambda} d\lambda} \mathbb{I}(0 \leq \lambda \leq 100)$$

looks a lot
like Gamma!



Numeric Inteyration.

$$x_i \sim \text{pois}(25), \quad E[x_i] = 25$$

$$\sum x_i \approx 625$$

$$\lambda^{625}$$



issues w/
overflow

$$\lambda = (0, 100)$$

$$\underline{100}^{625}$$

Introduction to Numeric Integration

Numeric Integration

- As we saw in the previous examples, one of the primary challenges of Bayesian estimation is the integration in the denominator of the posterior.
- Bayesian statistics has really exploded since the late 20th century, largely thanks to improved computational tools that help with the numeric integration.
- For this set of lectures, we only briefly introduce this topic. Depending on time and interest, we can explore this topic more later in the semester. /

Numeric Integration II

- For univariate functions, there are numerous approaches to well-approximate an integral.
- Traditional approaches are very simply, and are often based on Riemann-sum approximations.
- In R, one reliable function is the integrate function.
- Consider the integral $f(x) = x^2$,

$$\int_0^3 x^2 dx = 9$$

$$\frac{1}{3} x^3 \Big|_0^3 = 3^2 = 9$$

```
x_sq <- function(x) x^2
integrate(x_sq, lower = 0, upper = 3)
```

9 with absolute error < 1e-13

0.0000000000000001

Numeric Integration III

- Let m be the number of points used to evaluate the integral:

$$\int_A f(x) dx.$$

- If x is univariate, then the approach above is to take m points and do a numeric approximation.
- The standard Riemann approximation can be shown to converge to the true value at rate $O(1/m)$ for univariate functions, and can even be improved to faster rates (Liu and Liu, 2001, Chapter 1).
- However, these approaches scale very poorly as the dimensions of x and the integration area A increase.

Numeric Integration IV

- For instance, suppose that A is a 10-dimensional area (not even that large). Then, in order to achieve the $O(1/m)$ promised rate, you need to evaluate $O(m^{10})$ different points!

- 
- The primary alternative approach is known as **Monte Carlo** approximation.

Numeric Integration V

- Let $f(x; \theta)$ denote a pdf of some random variable, X . Then, if I is the integral

$$I = \underline{E[g(x)]} = \int_A g(x) f(x; \theta) dx,$$

$X \sim f(x; \theta)$
 $E[X] = \int_A x f(x) dx$

then the law of large numbers states that

$$E[g(x)] = \int g(x) f(x) dx$$

$$\hat{I}_m = \frac{1}{m} \sum_{i=1}^m g(X_i) \xrightarrow{a.s.} I,$$

where X_i is sampled from the distribution with density $f(x; \theta)$.

Numeric Integration VI

- Because we have an average of samples, the CLT gives us a way to approximate the error:

$$\sqrt{m}(I_m - I) \xrightarrow{d} N(0, \sigma^2),$$

where $\sigma^2 = \text{Var}(g(X))$.

$$O\left(\frac{1}{\sqrt{m}}\right)$$

- Thus, the error rate of the Monte-Carlo method is $O(m^{-1/2})$, regardless of the dimension of A . *Univariate: $O(1/m)$*
- The most common integral of this type is by letting f be uniform over the area A , in which case $f(x) = \frac{1}{|A|}$, and

$$I = \int_A g(x) dx,$$

$$I_m = \frac{|A|}{m} \sum_{i=1}^m g(X_i), \quad X_i \sim \text{Uniform}(A).$$

$$f(x) = \frac{1}{|A|}$$

$$\int g(x) dx = |A| \int g(x) f(x) dx$$

$$f(x) = O(g(x))$$

$$\lim_{x \rightarrow \infty} \frac{f(x)}{g(x)} = c$$

$$\hat{I} = I + \underline{O}\left(\frac{1}{\sqrt{m}}\right) \quad \text{Big-O}$$

$$\hat{I} - I = O\left(\frac{1}{\sqrt{m}}\right), \Rightarrow \lim_{m \rightarrow \infty} \frac{\hat{I} - I}{\left(\frac{1}{\sqrt{m}}\right)} = c$$

little-o
(faster).

$$\frac{\hat{I} - I}{\frac{1}{\sqrt{m}}} = o$$

$O_p(X_n)$



O_p

O_p

\approx

same,
convergence
in
prob.

Numeric Integration VII

- If x is univariate, this approach is worse than standard deterministic approaches $O(\underline{\underline{1/m}})$, but it has better performance in higher dimensional settings.

$$\int g(x) dx, \quad x \in \mathbb{R}$$

Numeric Integration VIII

- Example: $f(x) = x^2$ on the region $A = [0, 3]$

$$\int_0^3 x^2 dx$$

```
set.seed(12345)
```

```
m <- 10000
```

```
X <- runif(n = m, 0, 3)
```

```
3 * mean(x_sq(X))
```

```
[1] 8.992983
```

Monte-Carlo Replicates, particles

- Using the CLT, we can get a standard error of this estimate.

$\text{Var}(3X^2) = 64.8$, and therefore:

$$SE \approx \sqrt{\frac{64.8}{m}}$$

$$\begin{aligned} \int_0^3 x^2 dx &= \frac{1}{3} \int_0^3 x^2 dx \\ &= \frac{1}{3} E[x^2], \quad X \sim \text{Uniform}(0, 3) \end{aligned}$$

Numeric Integration IX

```
sqrt(64.8/m)
```

```
[1] 0.08049845
```

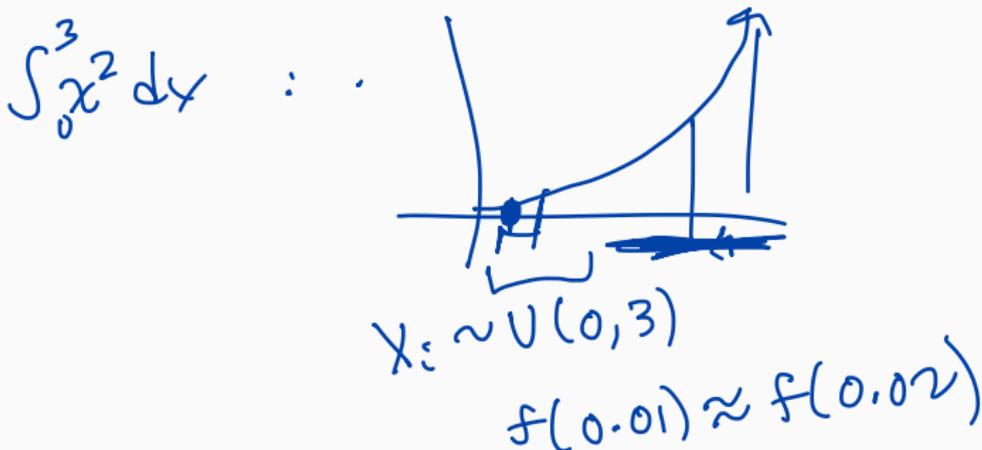
```
# Numeric Approximation:
```

```
sd(3 * X^2) / sqrt(m)
```

```
[1] 0.07999898
```

Numeric Integration X

- Theoretically, the Monte-Carlo approximation converges at a rate $O(m^{-1/2})$. There are two primary problems:
 1. The numerator in finite-sample approximations of the variance σ^2/m might be very large.
 2. Drawing uniform samples from A might be hard.
- The solution to these two problems is more advanced Monte-Carlo designs. We'll introduce **importance sampling**.

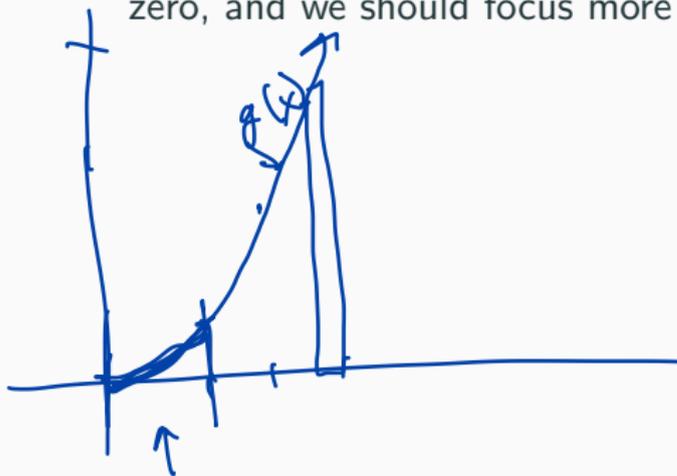


Numeric Integration XI

- Idea: not intervals of x contribute equally the function $f(x)$ and it's integral.

$$\int g(x)f(x)dx, \text{Var}(g(x))$$

- For instance, if $f(x) = x^2$, then values of x close to zero mean that the function $f \approx 0$. However, values of x near 3 have larger influence on the integral evaluation.
- Because of this, we don't need lots of samples from x near zero, and we should focus more on samples near 3.



Numeric Integration XII

- We can do this mathematically:

$$\rightarrow \int \underline{g(x)} \underline{f(x)} dx = \underbrace{E_{X \sim f(x)}} [\underline{g(X_i)}] \approx \underbrace{\frac{1}{m} \sum_{i=1}^m g(X_i)},$$

which is the same as

$$\int \frac{g(x)f(x)}{\pi(x)} \underline{\pi(x)} dx = \underbrace{E_{X \sim \pi(x)} \left[\frac{g(X)f(X)}{\pi(X)} \right]}_{\approx \frac{1}{m} \sum_{i=1}^m \frac{g(X_i)f(X_i)}{\pi(X_i)}}.$$

- The above approximation looks more complicated, but it has several advantages.
- The ratio $f(X_i)/\pi(X_i) = w_i$ is called the **importance weight**.

Numeric Integration XIII

- Now an important part of this is picking an appropriate sampling distribution $\pi(x)$.
- There is no “correct” way to do this, other than we want to have more samples that are concentrated in more “important” regions.
- We’ll look at a couple concrete examples to make this more clear.

Importance Sampling, Example 1

- Consider approximating the integral:

$$3 \cdot \int_0^3 x^2 \frac{1}{3} dx = \int_0^3 x^2 dx = 9$$

$\underbrace{\hspace{10em}}_{E[X^2] f(x)}$

$$= 3 \cdot E[X_i^2] \approx \frac{3}{m} \sum_{i=1}^m X_i^2$$

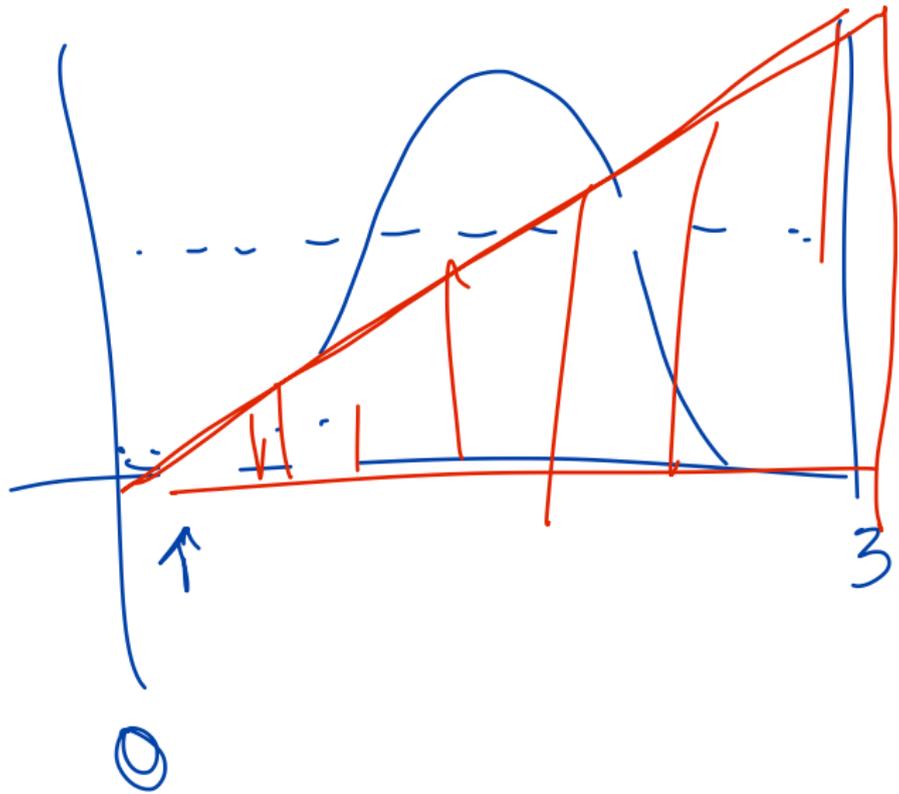
- We did the standard Monte-Carlo approach, using Uniform(0, 3) random variables:

```
set.seed(12345)
m <- 10000
X <- runif(n = m, 0, 3)
3 * mean(x_sq(X))
[1] 8.992983
```

Importance Sampling, Example 1 II

- We numerically approximated the standard error of this estimate to be:

```
# Numeric Approximation:  
sd(3 * X^2) / sqrt(m)  
[1] 0.07999898
```



Importance Sampling, Example 1 III

- Now let's try importance sampling. We don't want many low-values of X , and values should be between 0-3. Let's let $B_i \sim \text{Beta}(\alpha, \beta)$, and then $X_i = 3B_i$.
- After some checking, a good distribution might be:

$$X_i \sim 3 \times \text{Beta}(2, 1)$$

- A quick change-of-variables application gives:

$$\begin{aligned}\pi(x) &= \frac{1}{3} \frac{(x/3)^{\alpha-1} (1-x/3)^{\beta-1}}{B(\alpha, \beta)}, \quad x \in [0, 3] \\ &= \frac{1}{3} \frac{(x/3)}{B(2, 1)}, \quad x \in [0, 3] \\ &= \frac{2}{9}x, \quad x \in [0, 3]\end{aligned}$$

Importance Sampling, Example 1 IV

- Now that we have a sampling distribution $\pi(x)$, there are two different ways to think about the problem. The first is just a direct integral:

$$\int g(x) dx = \int \frac{g(x)}{\pi(x)} \pi(x) dx = E_{X \sim \pi(x)} \left[\frac{g(X)}{\pi(X)} \right],$$

or via the “target” distribution $f(x)$ approach:

$$\begin{aligned} \int \frac{g(x)f(x)}{\pi(x)} \pi(x) dx &= E_{X \sim \pi(x)} \left[\frac{g(X)f(X)}{\pi(X)} \right] \\ &\approx \frac{1}{m} \sum_{i=1}^m \frac{g(X_i)f(X_i)}{\pi(X_i)}. \end{aligned}$$

Importance Sampling, Example 1 V

- Both are correct, and sometimes the second is a useful way to think about a problem.
- In this case, the first approach is obvious, and the second approach we would pick the target distribution f to correspond to a $\text{uniform}(0, 3)$ distribution.
- Thus, approximating the integral:

```
m <- 10000
```

```
X <- 3 * rbeta(n = m, 2, 1)
```

```
pi_x <- function(x) 2*x/9
```

```
mean(x_sq(X)/pi_x(X))
```

```
[1] 8.993616
```

$$= \frac{1}{m} \sum \frac{g(x)}{\pi(x)} \approx \int \frac{g(x) \pi(x)}{\pi(x)} dx$$

$$= \int g(x) dx$$

Importance Sampling, Example 1 VI

- We can once again get an estimate of the standard error using the CLT:

$$SE \approx \frac{\sigma_{w_i}^2}{\sqrt{m}},$$

where w_i is the importance weight.

```
sd( (X^2) / (2 * X / 9) ) / sqrt(m)
[1] 0.03181511
```

This error was about half of the default Monte-Carlo method.

Importance Sampling, Example 1 VII

- This example is a bit trivial, because the integral is not hard to compute.
- Also, our choice of sampling distribution meant we could get a closed-form solution for sampling weights:

$$\begin{aligned} \pi(x) &= \frac{2}{9} \times \mathbb{1}(0 \leq x \leq 3) \\ \hat{I}_m &= \frac{1}{m} \sum_{i=1}^m \frac{X^2}{\frac{2X}{9}} \\ &= \frac{1}{m} \sum_{i=1}^m \frac{9X}{2} \\ &= \frac{9}{2} \bar{X}. \end{aligned} \quad \hat{I} = \frac{1}{m} \sum \frac{g(x)}{\pi(x)}$$

Importance Sampling, Example 1 VIII

- We could actually simplify this even further by picking a Beta(3, 1) sampling distribution:

$$\begin{aligned}\pi(x) &= \frac{1}{3} \frac{(x/3)^{\alpha-1} (1-x/3)^{\beta-1}}{B(\alpha, \beta)}, \quad x \in [0, 3] \\ &= \frac{1}{3} \frac{(x/3)^2}{B(3, 1)}, \quad x \in [0, 3] \\ &= \frac{1}{9} x^2, \quad x \in [0, 3]\end{aligned}$$

$$\begin{aligned}\hat{I} &= \frac{1}{m} \sum \frac{g(x)}{\pi(x)} \\ &= \frac{1}{m} \sum \frac{x^2}{(\frac{1}{9} x^2)} = 9 \frac{1}{m} \cdot m \\ &= 9\end{aligned}$$

Importance Sampling, Example 1 IX

- Thus, if we picked this distribution, we could actually get the exact answer!

$$\begin{aligned} I_m &= \frac{1}{m} \sum_{i=1}^m \frac{X^2}{9} \\ &= \frac{9}{m} \sum_{i=1}^m 1 \\ &= 9. \quad = \perp \end{aligned}$$

- This leads us to the identity that if $\pi(x) \propto g(x)$, such that $\underline{g(x) = c\pi(x)}$, then the integral is:

$$\underline{\int g(x) dx} = \int \left(\underline{g(x)/\pi(x)} \right) \pi(x) dx = c \int \pi(x) dx = \underline{c}$$

Importance Sampling, Example 1 X

- This effectively never happens in real world-scenarios, because if it did there wouldn't be a reason to do Monte-Carlo.
- However, it does help us decide a useful principle: try to pick a $\pi(x)$ such that $\pi(x) \propto g(x)$ as much as possible.

Importance Sampling, Example II

Importance Sampling: extreme events

If $Z \sim N(0, 1)$, approximate the probability:

$$P(Z > 3) = I = \int_3^{\infty} \frac{1}{2\sqrt{\pi}} e^{-x^2/2} dx.$$
$$= \int_{-\infty}^{\infty} \mathbb{1}_{(3 < x)} \frac{1}{2\sqrt{\pi}} e^{-x^2/2} dx$$

- Once again, we have an exact method to calculate the integral, so we can see how good our approximation is:

Actual value

`1-pnorm(3)`

[1] 0.001349898

$$= 1 - P(Z \leq 3) = \underline{P(Z > 3)}$$

Importance Sampling, Example II II

- We can use indicator functions to help write this in the standard Monte-Carlo form:

$$h(x) = I(x > 3),$$

then

$$I = \int_3^{\infty} \frac{1}{2\sqrt{\pi}} e^{-x^2/2} dx = \int_{-\infty}^{\infty} h(x) \frac{1}{2\sqrt{\pi}} e^{-x^2/2} dx.$$

Handwritten notes: "pdf" with an arrow pointing to the integrand; "g(x)f(x)dx" with arrows pointing to h(x) and the integrand; "= E[h(x)]" with an arrow pointing to the integral; "if X ~ N(0,1)" written below.

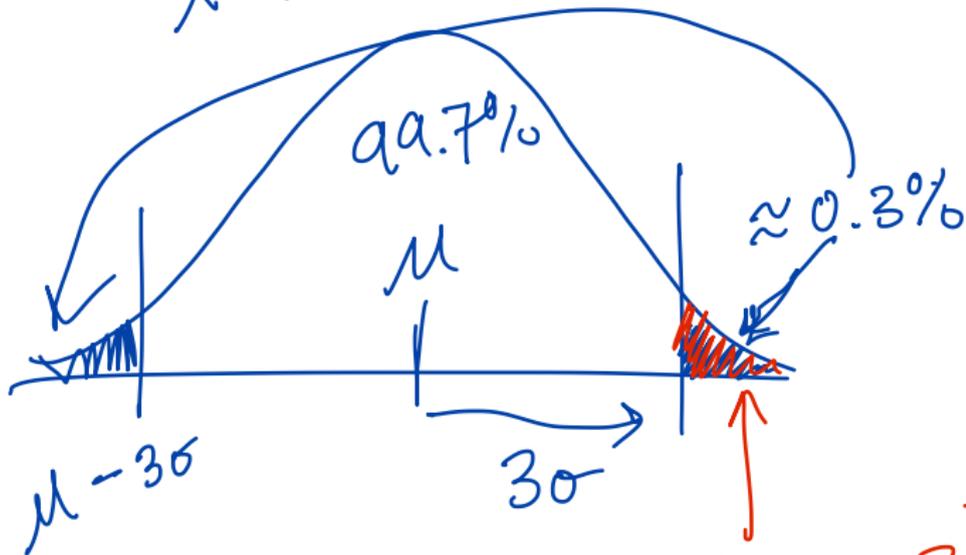
- Thus, the standard Monte-Carlo approach may be:

$$\hat{I}_m = \frac{1}{m} \sum_{i=1}^m h(X_i), \quad X_i \sim N(0, 1).$$

Handwritten: A bracket under the sum in the equation above points down to " \hat{p} , prop $X_i > 3$."

$$X \sim N(\mu, \sigma^2)$$

68 - 95 - 99.7



$$P(Z > 3)$$

$$\approx 0.15\%$$

$$P = \underline{\underline{0.0015}}$$

Importance Sampling, Example II III

```
m <- 10000
X1 <- rnorm(n = 10000)
h <- function(x) ifelse(x > 3, 1, 0)

mean(h(X1))
[1] 0.0013
```

- Because $h(X_i)$ is binary, the standard error is:

$$SE \approx \sqrt{\frac{\hat{I}_m(1 - \hat{I}_m)}{m}}$$

```
sqrt(mean(h(X1)) * (1 - mean(h(X1))) / m)
[1] 0.0003603207
```

Importance Sampling, Example II IV

- The problem with this approach, however, is that if the $X_i \sim N(0, 1)$, then almost none of the samples will be larger than 3 (very rare event), so the estimate is high-variance!
- That is, we will end up with $h(X_i) = 0$ for **nearly all** samples of X_i .
- We want to focus our samples in the “important” regions to reduce variance.
- Thus, consider instead sampling from $\pi(x) \sim N(4, 1)$, so we have more weight in the important part. Then:

$$\hat{I}_m = \frac{1}{m} \sum_{i=1}^m h(X_i) \frac{f(X_i)}{\pi(X_i)}, \quad X_i \sim N(4, 1).$$

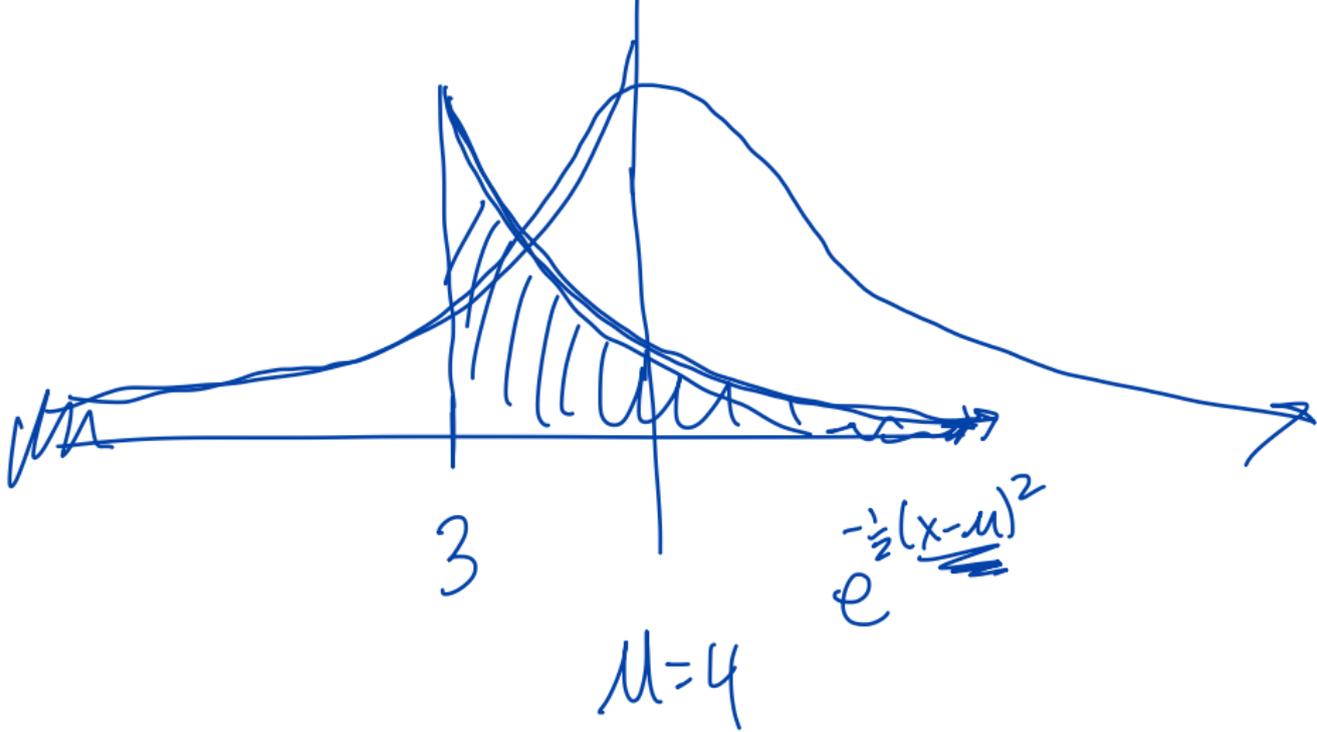
$$I = \int_3^{\infty} \phi(x) dx = \int_{-\infty}^{\infty} h(x) \phi(x) dx$$

$$\approx \frac{1}{m} \sum h(x_i), \quad x_i \sim \mathcal{N}(0,1)$$

$$= \int_3^{\infty} \phi(x) dx = \int_{-\infty}^{\infty} h(x) \phi(x) dx$$

$$= \int_{-\infty}^{\infty} h(x) \phi(x) \frac{\pi(x)}{\chi(x)} dx$$

$$\approx \frac{1}{m} \sum h(x_i) \phi(x) \pi(x) / \chi(x), \quad x_i \sim \pi(x) = \mathcal{N}(4,1)$$



Importance Sampling, Example II V

```
X2 <- rnorm(m, mean = 4)
weights2 <- dnorm(X2) / dnorm(X2, mean = 4)
mean(h(X2) * weights2)
[1] 0.001326697
```

$$\frac{f(x)}{\pi(x)} \begin{matrix} \nearrow \phi(x) \\ \nwarrow \phi(x-4) \end{matrix}$$

- This time, the standard error is given numerically by:

$$\underline{SE} \approx \frac{sd(h(X_i)w_i)}{\sqrt{m}}$$

```
sd(h(X2)*weights2) / sqrt(m)
```

```
[1] 3.047903e-05
```

.0000305 ← importance
.0003... ← vanilla MC

$$g(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

~~$x > 3,$~~

$$e^{-\frac{1}{2}3^2}$$

$$e^{-\frac{9}{2}}$$

Importance Sampling, Example II VI

- There is an issue that many of the sampled X_i values are less than 3, so we might want to try a completely different sampling approach.
- Consider the function $g(x)$, when $x > 3$, then $g(x) \propto e^{-9}$.
- Thus, we might consider sampling X_i such that:

$$X_i \sim 3 + \text{Exp}(9)$$

- We again need to do a variable transformation, but this one is easy. If $Y \sim \text{Exp}(\lambda)$, then for $X = Y + 3$,

$$\pi(x) = f_y(x - 3).$$

Importance Sampling, Example II VII

```
X3 <- 3 + rexp(m, 9)
weights3 <- dnorm(X3) / dexp(X3-3, 9)
mean(h(X3) * weights3)
[1] 0.001303543
```

Importance Sampling, Example II VIII

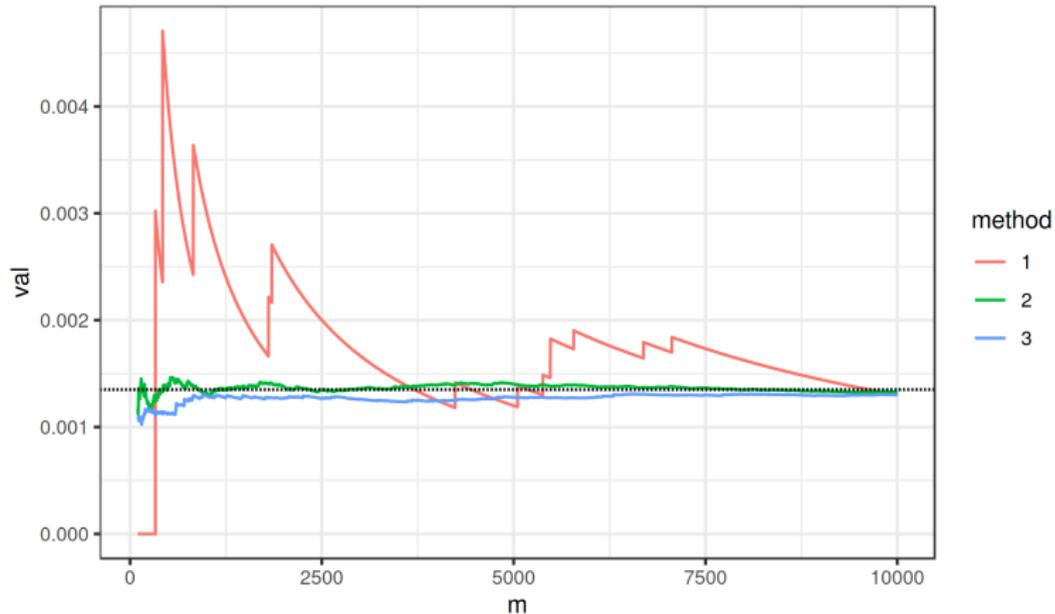
- Finally, let's compute these 3 different estimate for every value of $m \in \{2, 3, \dots, 10000\}$.

Importance Sampling, Example II IX

```
library(ggplot2)
est1 <- cumsum(h(X1)) / 1:m
est2 <- cumsum(h(X2) * weights2) / 1:m
est3 <- cumsum(h(X3) * weights3) / 1:m
all_vals <- data.frame(
  val = c(est1, est2, est3),
  method = rep(1:3, each = m) |> factor(),
  m = rep(1:m, 3)
)

ggplot(all_vals |> dplyr::filter(m > 100), aes(x = m, y = val)) +
  geom_line() +
  geom_hline(yintercept = 1-pnorm(3), linetype = 'dashed') +
  theme_bw()
```

Importance Sampling, Example II X



$X_i \stackrel{iid}{\sim} \text{Pois}(\lambda)$, $\Delta \sim \text{Uniform}(0, 100)$

$$f_{\Delta|X}(\lambda/x^*) = \frac{\lambda^{\sum x_i^*} e^{-n\lambda}}{\int_0^{100} \lambda^{\sum x_i^*} e^{-n\lambda} d\lambda} \cdot \mathbb{I}(0 \leq \lambda \leq 100)$$

$X_i \sim \text{Pois}(25)$, $n=25$, $\sum X_i \approx \underline{\underline{\underline{625}}}$
 $\approx \lambda^{625}$

$$S = \sum X_i^* \quad f(\lambda) = \frac{\lambda^S e^{-n\lambda}}{\int_0^{100} \lambda^S e^{-n\lambda} d\lambda}$$

We want $\int_0^{100} f(\lambda) d\lambda$.

$$\int_0^{100} \exp(\log(f(x))) dx$$

$$\exp(\log(f(x))) = \exp(S \log(x) - n \lambda)$$

$$e^{625 \log(\lambda) - n \lambda}$$

\downarrow 0-100
 ≈ 100 - 100

$$g(x) = S \log x - n x$$

$$g'(x) = \frac{S}{x} - n = 0$$

$$\Rightarrow \arg \max_x g(x) = \frac{S}{n}$$

$$f(x) = \exp(g(x))$$

$$f(x) = \exp(g(x) - g(\bar{x}) + g(\bar{x}))$$

$$\rightarrow \left[= \underbrace{\exp(g(\bar{x}))}_{\uparrow} \exp(g(x) - g(\bar{x})) \right]$$

$$f(\lambda|x) = \frac{\lambda^s e^{-n\lambda} \mathbb{1}(0 \leq \lambda \leq 100)}{\int_0^{100} \lambda^s e^{-n\lambda} d\lambda}$$

$$E[A|X] = \frac{\int_0^{100} \lambda \cdot \lambda^s e^{-n\lambda} d\lambda}{\int_0^{100} \lambda^s e^{-n\lambda} d\lambda} = \frac{\int_0^{100} \lambda^{s+1} e^{-n\lambda} d\lambda}{\int_0^{100} \lambda^s e^{-n\lambda} d\lambda}$$

$$= \frac{\cancel{\exp(g(\bar{x}))} \cdot \int_0^{100} \lambda \cdot \exp(g(x) - g(\bar{x})) d\lambda}{\cancel{\exp(g(\bar{x}))} \cdot \int_0^{100} \exp(g(x) - g(\bar{x})) d\lambda}$$

$$= \frac{\int_0^{100} \lambda \exp(g(x) - g(\bar{x})) d\lambda}{\int_0^{100} \exp(g(x) - g(\bar{x})) d\lambda}$$

denom = integrate (

f = function(x) exp(g(x) - \bar{g}),

lower = 0

upper = 100

March 3rd recap

- Bayesian estimation

$$\pi(\theta | x^*) = \frac{f(x^*; \theta) \pi(\theta)}{\int f(x^*; \theta) \pi(\theta) d\theta}$$

→ conjugate prior,

- makes integral "easy"
- we already know the answer, just look up conjugate prior table.

- Numeric Integration

univariate method in R:

- integrate (f, lower, upper)

↓
 $\int_{\text{lower}}^{\text{upper}} f(x) dx$

- Pois(x) likelihood, $\lambda \sim U(0, 100)$

den: $\int_{\underline{\lambda}}^{\infty} \lambda^{\sum x_i} e^{-n\lambda} d\lambda$, $\sum x_i \approx 600^+$

- Monte-Carlo integration:

Idea: Expected Values are
integrals, Sample means converge
to Expected Values.

$$\int f(x) dx = \int f(x) \frac{\pi(x)}{\pi(x)} dx = E \left[\frac{f(X)}{\pi(X)} \right]$$

$$\approx \frac{1}{m} \sum_{i=1}^m \frac{f(x_i)}{\pi(x_i)} \quad \text{if } X \sim \pi(x)$$

$$\int \underline{h(x)} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} dx \approx \frac{1}{m} \sum_{i=1}^m h(x_i),$$

$$x_i \sim \mathcal{N}(0, 1)$$

$$\int h(x) \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} \cdot \frac{\pi(x)}{\pi(x)} dx \approx \frac{1}{m} \sum_{i=1}^m \frac{h(x_i) \phi(x_i)}{\pi(x_i)}$$

" "

$$\int h(x) \phi(x) dx$$

$$\boxed{X \sim \pi(x)}$$

Rejection Sampling

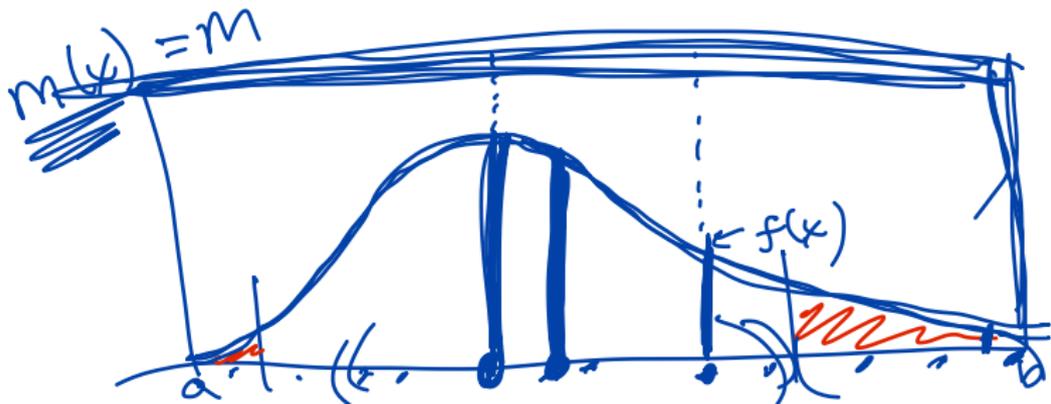
- We can now see some recurring themes in Bayesian computing (and more generally, approximating integrals).
- For Monte-Carlo integral calculations, we first need to find an appropriate distribution to get samples $X_i \sim \pi(x)$, then apply importance sampling.
- Often, there's not an obvious choice for π , or we can't directly sample from $\pi(x)$.
- In many cases, we can do **rejection sampling** to get samples from $\pi(x)$, as discussed last semester.

* 6.2

Math 4450 notes

- Say we want to sample from $f(x)$. $r \sim \text{dist}$ ($n = \# \text{ samples}, \theta$)

$f(x)$ has support on $[a, b]$



$M(x)$ - bounds $f(x)$

$$\underline{M}(x) \leq \underline{f}(x) \leq 0$$

$$m(x) = \frac{M(x)}{\int M(x) dx}$$

$m(x)$ is a pdf.

draw samples from $m(x)$

(1) draw $T \sim m(x)$

(2) draw $U \sim U(0,1)$, independent
of T .

$$U \leq \frac{f(T)}{m(T)}$$

then

"accept"

else, "reject"

$$T_{(\text{accept})} \sim \underline{f(x)}$$

Variance reduction techniques

- We won't go into a lot of details here, but there are some approaches highlighted in Liu and Liu (Section 2.3 of 2001) that can help with Monte-Carlo evaluations.
- One of the main problems is the variance σ^2 that arises in the numerator. These approaches are intended to reduce the variance, while not adding any bias.

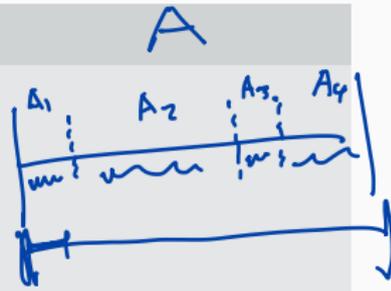
→ importance sampling.

Variance reduction techniques II

Stratified Sampling

Suppose we wish to calculate the integral

$$\int_A f(x) dx.$$



Using Monte-Carlo sampling, the variance is σ^2/n , where σ^2 is the variance of the function f over the domain A .

Instead, consider breaking the domain A into distinct areas: A_1, A_2, \dots, A_k , such that the variance of f over these areas is roughly constant, then get Monte-Carlo samples from these regions independently.

A_i , m_i samples

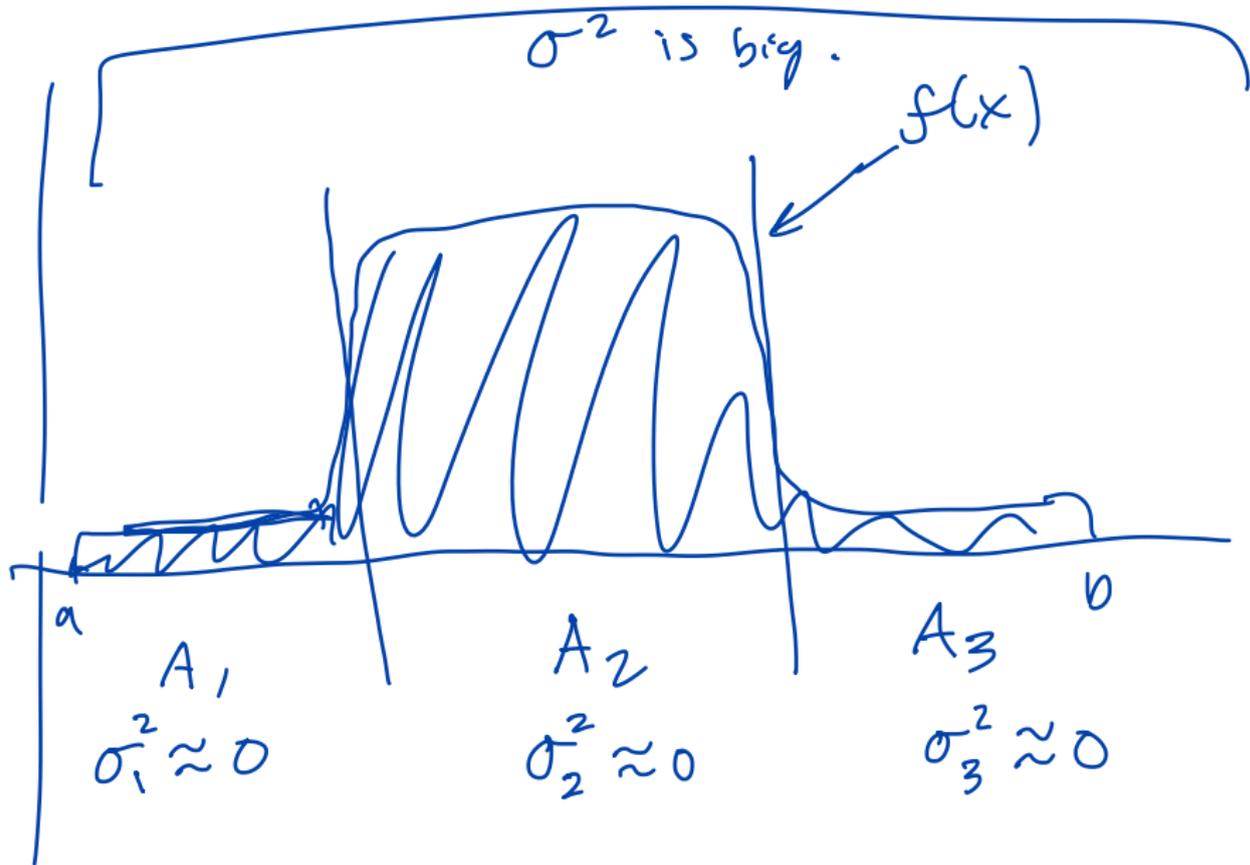
$$\mu_i = \int_{A_i} f(x) dx \approx \frac{1}{m_i} \sum_{j=1}^{m_i} f(x_{i,j}) = \hat{\mu}_i$$

$$X_{i,j} \sim U(A_i)$$

$$\int_A f(x) dx \approx \sum_{i=1}^K \hat{\mu}_i$$

M.C.

$$\text{Var}(\hat{\mu}) = \sum_{i=1}^K \frac{\sigma_i^2}{m_i} \leq \left[\frac{\sigma^2}{m} \right]$$



Variance reduction techniques III

Control Variates Method

In this method, one uses a control variate C which is correlated with the sample X , to produce a better estimate.

Suppose we want to estimate $\mu = E[X]$, and $\mu_C = E[C]$ is known. Then, we can produce Monte Carlo samples of the form:

$$X_i^* = X_i - b(C - \mu_C).$$

$$\mu = \int x f(x) dx \approx \frac{1}{m} \sum X_i, \quad X \sim f(x)$$

$$\frac{1}{m} \sum (X_i - b(C - \mu_C))$$

$$E[X_i^*] = E[X_i - b(C - \mu_c)]$$

$$= E[X_i] - b \underbrace{E[C - \mu_c]}_0$$

$$E[X_i^*] = E[X_i]$$

$$\left. \begin{aligned} \text{Var}(X_i^*) &= \text{Var}(X_i) - 2b \text{Cov}(X_i, C) \\ &\quad + b^2 \text{Var}(C) \end{aligned} \right\}$$

always a choice b , s.t.

$$\text{Var}(x_i^*) \leq \text{Var}(x_i).$$

$$\rightarrow b = \frac{\text{cov}(x, c)}{\text{Var}(c)}$$

$$\begin{aligned} \text{Var}(x_i^*) &= (1 - \rho_{xc}^2) \text{Var}(x_i) \\ &\leq \text{Var}(x_i) \end{aligned}$$

$$X_i \sim N(0,1)$$

$$E[e^{X_i}] = \mu = m(1) = e^{-1/2}$$

$$\hat{\mu} = \frac{1}{m} \sum e^{X_i}, \quad X_i \sim N(0,1).$$

C_i correlated with e^{X_i}

$$\underline{C_i = X_i.}$$

$$\hat{b} = \frac{\text{cov}(e^{x_i}, x_i)}{\text{var}(x_i)} = \underline{\underline{\text{cov}(e^{x_i}, x_i)}}$$

$$X_i \sim \text{rnorm}(m, 0, 1)$$

$$\hat{b} = \text{cov}(\exp(x), x)$$

$$X_i^* = e^{x_i} + \hat{b}(x_i - 0)$$

$$= \underline{e^{x_i}} + \underline{\underline{\text{cov}(e^{x_i}, x_i) X_i}}$$

$$\uparrow \text{var}(x_i^*) \leq \text{var}(x_i)$$

Variance reduction techniques IV

Antithetic Variates Method

Suppose we want to compute an integral $\int_0^1 f(x)dx$. We can sample $U_i \sim U(0,1)$, and do Monte-Carlo as usual with $f(U_i)$. However, if f is monotonic, then $U_i' = 1 - U_i$ is **antithetic** to U_i , and

$$\frac{1}{m} \sum f(u_i)$$

$$\text{Cov}(U_i, 1 - U_i) = -\text{Var}(U_i).$$

Thus, for every sample $U_i \sim U(0,1)$ drawn, calculate instead:

$$\int_0^1 f(x)dx \approx \frac{1}{m} \sum_{i=1}^m (f(u_i) + f(1 - u_i))/2$$

$$X_i \sim F_{\frac{1}{2}} \text{ cdf,}$$

then $U_i \sim U(0,1)$,

$$\underline{\underline{X_i = F^{-1}(U_i)}},$$

$$X_i \sim F$$

$$X_i = F^{-1}(U_i),$$

antithetic sample. X_i' is just

$$\begin{aligned} X_i' &= F^{-1}(1 - U_i) \\ &= F^{-1}(U_i') \end{aligned}$$

$$\int f(x) dx = \frac{1}{m} \sum_{i=1}^m \frac{f(x_i) + f(x'_i)}{2}$$

monotone

$$\int_0^{\infty} g(x) \cdot e^{-x} dx.$$

$$\approx \frac{1}{m} \sum_{i=1}^m g(x_i)$$

$$x_i \sim \text{exp.}$$

$$F^{-1}(x) = -\ln(1-x)$$

$$e^{-x} = f(x) \text{ is } \text{exp}(1)$$

$$U_i \sim U(0,1)$$

$$X_i = -\log(U_i) \sim \text{exp}(1)$$

$$\int_0^{\infty} g(x) e^{-x} dx \approx \frac{1}{m} \sum_{i=1}^m \frac{g(-\log(U_i)) + g(-\log(1-U_i))}{2}$$

Pois(λ), $X_i \stackrel{iid}{\sim}$ Pois(λ)

$E[\mathbb{1}|X]$

$\lambda = 25$

10000

$\hat{\lambda} \approx 25$ -

$\lambda = 24.5$,

$\lambda = 25.5$

10^{-6}

X_1, X_2, \dots, X_{25}

Y_1, Y_2, \dots, Y_{25}

10^{-3}

24.89999

practically
= 24.9

rate of convergence "integrate"

$$O\left(\frac{1}{m}\right), \quad m = \# \text{ points}$$

Monte Carlo : $O\left(\frac{1}{m^{1/2}}\right)$

$$\frac{\sigma^2}{\sqrt{m}} \leftarrow \text{unknown.}$$

Review 4/10

$\pi(\theta) \leftarrow$ prior belief

$L(\theta) \leftarrow$ likelihood,

$$X \sim L(\theta)$$

$$X_i \stackrel{\text{iid}}{\sim} f(x_i; \theta)$$

$\theta|X \leftarrow$ posterior dist'n.

$$\pi(\theta|x) = \frac{L(\theta)\pi(\theta)}{\int_{\tau} L(\tau)\pi(\tau)d\tau} . \quad]$$

$$\hat{\theta}_{\text{MAP}} = \underset{\theta}{\operatorname{argmax}} \pi(\theta|x), \quad \text{Maximum a Posteriori.}$$

$$\hat{\theta}_{\text{Posterior Mean}} = E[\theta|x]$$

$$\hat{\theta}_{\text{PM}} = \int \theta \pi(\theta|x) d\theta$$
$$= \left[\frac{\int \theta L(\theta) \pi(\theta) d\theta}{\int L(\tau) \pi(\tau) d\tau} \right] \leftarrow$$

Choice of Priors

$X \sim \text{Bin}(n, \theta)$, $\theta = \text{prob of H.}$

$\theta \sim U(0,1)$

log-odds $\tau = \log \frac{\theta}{1-\theta}$

$\pi(\tau)$ is not uniform.

$g(\theta) | X$

it depends on choice of prior, but also g .

Jeffrey's priors

- A common safe-choice for a prior distribution is a uniform prior.
- However, there is some (not universal) belief that there is no such thing as a uniform prior.
- Consider the Binomial(N, p) data examples. A “uniform” prior for p might look like:

$$\pi(p) = 1(0 \leq p \leq 1).$$

- This Binomial model arises quite frequently in biomedical sciences. In this setting, we often are interested in the **log-odds**:

$$\theta = \log \left(\frac{p}{1-p} \right).$$

Jeffrey's priors II

- If we pick a uniform prior for p , what does the prior for θ look like?

$$\underline{p \sim U(0,1)}$$

$\theta = \log\left(\frac{p}{1-p}\right)$, what is
the prior for θ ?

$$0 \leq p \leq 1, \quad g(p) = \log \frac{p}{1-p}$$

is monotonic.

$$g^{-1}(\theta) = \frac{e^\theta}{1+e^\theta}$$

$$\frac{d}{d\theta} g^{-1}(\theta) = \frac{e^\theta}{(1+e^\theta)^2}$$

$$\pi_\theta(\theta) = \pi_p(g^{-1}(\theta)) \cdot \left| \frac{d}{d\theta} g^{-1}(\theta) \right|$$

$$= \mathbb{1}(0 \leq g^{-1}(\theta) \leq 1) \cdot \frac{e^\theta}{(1+e^\theta)^2}$$

$$= \frac{e^\theta}{(1+e^\theta)^2}$$

- invariance principle is broken.

→ $P \sim U(0,1)$.

~~P^{100}~~ close to zero.

- Jeffrey's prior : pick a prior,
so that the posterior

of any transformation
gives the same answer
↑
distribution.

$\Theta \xrightarrow{g} \Psi$, pick a prior so
that

$$\underline{\pi_{\Psi|x}(\Psi|x) = \pi_{\Theta|x}(\Theta|x)} .$$

Hierarchical Bayes

Hierarchical Bayes

- The idea behind Hierarchical Bayes is simple: our model f depends on parameters θ .
- We can get a prior for θ , $\pi(\theta)$.
- The prior itself depends on parameters, say $\pi(\theta; \theta_1)$.
- How do we choose θ_1 ? Sometimes we might know θ_1 , but sometimes not.
- In a pure Bayesian paradigm, if we don't know the value of θ_1 , then it is also a random variable Θ_1 , and we should put a prior on this as well!
- In some way, this allows us to be less-committal about the parameters in the prior model, and instead allow the data to inform our choice of priors (to some degree).

Hierarchical Bayes II

- Philosophically, this situation naturally arises if we want to pick a conjugate prior for Θ , but are not committal about the **hyperparameters** Θ_1 that define the distribution of Θ .
- We could continue doing this many times if we wanted!
- The prior for Θ_1 might depend on parameters θ_2 , which we model as a random variable Θ_2, \dots
- This leads to a model for $(X, \Theta, \Theta_1, \dots, \Theta_N)$.
- However, there is a conditional structure to this model:

$$\Theta_N \longrightarrow \Theta_{N-1} \longrightarrow \dots \longrightarrow \Theta \longrightarrow X.$$

- Thus, X depends only on Θ , and Θ_n only on Θ_{n+1} :

$$X|\Theta = \theta \sim f(x|\theta), \quad \Theta|\Theta_1 = \theta_1 \sim \pi_1(\theta|\theta_1) \quad \dots \quad \Theta_N \sim \pi_N(\theta_n).$$

Hierarchical Bayes III

- Using rules of marginal probability and conditional probability, then

$$\pi(\theta|x) \propto L(\theta) \pi(\theta)$$

$$\pi(\theta) = \int \pi(\theta, \theta_1, \dots, \theta_N) d\theta_{1:N}$$

$$= \int \pi(\theta|\theta_{1:N}) \pi(\theta_{1:N}) d\theta_{1:N}$$

$$= \int \pi(\theta|\theta_1) \pi(\theta_1|\theta_{2:N}) \pi(\theta_{2:N}) d\theta_{1:N}$$

$$= \vdots$$

$$= \int \pi(\theta|\theta_1) \pi(\theta_1|\theta_2) \dots \pi(\theta_{N-1}|\theta_N) \pi(\theta_N) d\theta_{1:N}$$

$$\pi(\theta) = \int \pi(\theta|\theta_1) \pi(\theta_1) d\theta_1$$

↑

Standard

Hierarchical Bayes IV

- Thus, the hierarchical model is functionally equivalent to the standard Bayesian model:

$$X|\Theta = \theta \sim f(x|\theta) \quad \Theta \sim \pi(\theta),$$

where $\pi(\theta)$ is given by the integral above.

- Why would we want to do this?
 1. Sometimes the data / problem give rise to a natural hierarchical structure, and this idea will be useful. Here, we might actually be interested in the hyperparameters $\theta_1, \dots, \theta_N$.
 2. We can now be less committal about our priors, while still using desirable structures.
 3. It can sometimes aid computations.

Hierarchical Bayes V

Trivial case: hierarchical Normal-Normal

Suppose that the data X_i are iid $N(\theta, 1)$. Set a prior for θ as $\Theta | \Theta_1 = \theta_1 \sim N(\theta_1, 1)$, and $\Theta_1 \sim N(0, 1)$.

What is distribution (or prior)
of θ .

$$\pi_{\theta}(\theta) = \int \pi_{\theta|\theta_1}(\theta|\theta_1) \pi_{\theta_1}(\theta_1) d\theta_1$$

$$\rightarrow = \int \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(\theta - \theta_1)^2} \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(\theta_1)^2} d\theta_1$$

$$= \frac{1}{2\sqrt{2\pi}} e^{-\frac{1}{2(2)^2}(\theta)^2}$$

$$\theta \sim \mathcal{N}(0, 2^2)$$

Hierarchical Bayes VI

More realistic example: Coin-toss experiment

Suppose your friend gives you a coin from another country, and you want to estimate $\theta = p$, the probability of heads. Thus, in N tosses, the natural model for X , the number of heads, $X \sim \text{Bin}(N, \theta)$. You believe that the proportion is close to $1/2$, but not quite sure. A nice prior would be the Beta(α, β)-distribution, since it is conjugate for the binomial family.

If $\Theta \sim \text{Beta}(\alpha, \beta)$, then $E[\Theta] = \frac{\alpha}{\alpha + \beta}$. Thus, if I want a prior centered at $1/2$, I can pick: $\theta_1 = \alpha = \beta$, and $E[\Theta] = \theta_1 / 2\theta_1 = 1/2$. We can now give a prior for Θ_1 .

Hierarchical Bayes (continued)

- For now, we will restrict our choices of Θ_1 to be integers.

```
Theta <- seq(1e-8, 1-1e-8, length.out = 1000)
```

```
B1 <- dbeta(Theta, 1, 1)
```

```
B2 <- dbeta(Theta, 2, 2)
```

```
B3 <- dbeta(Theta, 3, 3)
```

```
B5 <- dbeta(Theta, 5, 5)
```

```
B10 <- dbeta(Theta, 10, 10)
```

```
plot(x = Theta, y = B1, type = 'l', ylim = c(0, 3.5), col = "#c6
```

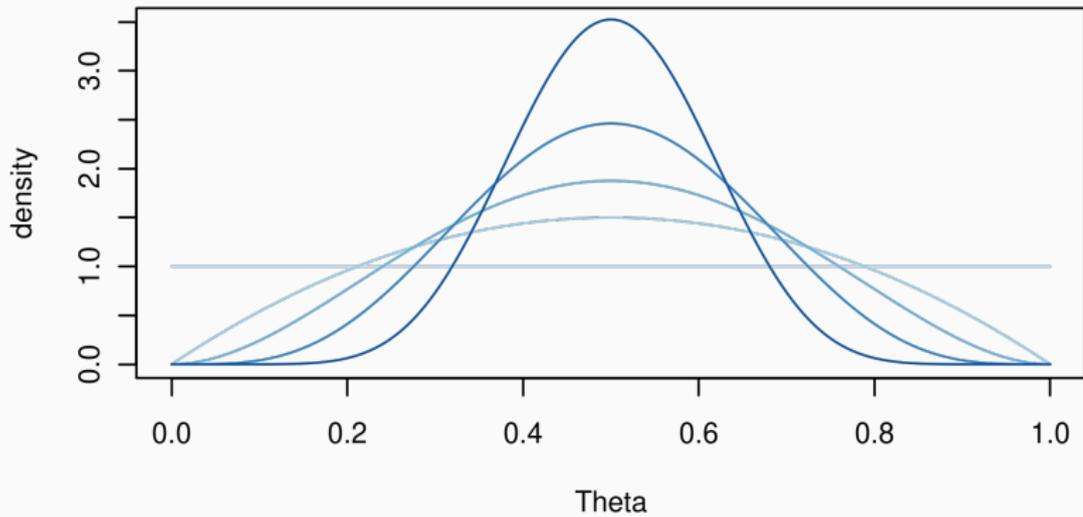
```
lines(x = Theta, y = B2, type = 'l', col = '#9ecae1')
```

```
lines(x = Theta, y = B3, type = 'l', col = '#6baed6')
```

```
lines(x = Theta, y = B5, type = 'l', col = '#3182bd')
```

```
lines(x = Theta, y = B10, type = 'l', col = '#08519c')
```

Hierarchical Bayes (continued) II



Hierarchical Bayes (continued) III

- As θ_1 grows, the variance of Θ shrinks at a rate $O(\theta_1)$.
- Thus, to be noncommittal about our prior on Θ , we will set a **hyperprior** on Θ_1 that has more weight on smaller values of k :

$$\rightarrow \pi_{\Theta_1}(k) = \frac{1}{2 \log(2) k(2k-1)}, \quad k \in \{1, 2, \dots\}$$

- This hyper-prior was selected somewhat out of convenience (The Catalan Numbers), which will allow us to get the marginal prior of Θ :

$$\pi(\theta) = \sum_{k=1}^{\infty} \pi_{\Theta|\Theta_1}(\theta|k) \pi_{\Theta_1}(k) = \frac{1 - |1 - 2\theta|}{4 \log(2) \theta(1 - \theta)}, \quad 0 < \theta < 1$$

proof / derivation is in
the notes.

Hierarchical Bayes (continued) IV

- In this case, we can get a closed-form expression for $\pi(\theta)$ but as you can tell, it can often get very difficult to do this mathematically.
- Thus, while the hierarchical structure is equivalent to just setting $\pi(\theta)$ as our prior (and not worrying about hierarchical model), this additional structure can aid in computations.
- If we are looking to estimate, for instance, the posterior mean:

$$E_{\Theta|X}[\Theta],$$

Then the law of total expectation gives:

$$E_{\Theta|X}[\Theta|X] = E_{\Theta_1|X} [E_{\Theta|\Theta_1,X}[\Theta|\Theta_1, X]].$$

$$E[Y] = E_z [E[Y|z]]$$

Hierarchical Bayes (continued) V

- Thus, the calculation of the posterior mean of $\Theta|X$ can be done without needing explicit form of the posterior $\Theta|X$, which can simplify the problem.
- Our particular choice of likelihood and prior makes it easy to calculate the marginal-likelihood of $\Theta_1 = k$:

$$\begin{aligned}\pi_{X|\Theta_1}(x|k) &= \int_0^1 f(x|\theta, k)\pi_{\Theta|\Theta_1}(\theta; k) d\theta \\ &= \binom{N}{x} \frac{B(x+k, N-x+k)}{B(k, k)}.\end{aligned}$$

- Also, The Beta distribution was picked because it is conjugate, so the posterior mean $\Theta|\Theta_1 = k, X$ is readily available:

$$E_{\Theta|\Theta_1=k, X} = \mu_k = \frac{x+k}{N+2k}.$$

Hierarchical Bayes (continued) VI

- Now we need to take the expectation of this, with respect to the marginal posterior (un-normalized weights) $\pi_{\Theta_1|x}(k|x)$:

$$\begin{aligned}\pi_{\Theta_1|x}(k|x) &\propto \underline{w_k} \\ &= \pi_{X|\Theta_1}(x|k)\pi_{\Theta_1}(k) \\ &= \frac{B(x+k, N-x+k)}{2\log(2)B(k,k)k(2k-1)}.\end{aligned}$$

- Then, the normalized weights are:

$$\bar{w}_k = \frac{w_k}{\sum_j w_j} = p(k|x),$$

and the posterior mean is:

$$E[\Theta|x] = \sum_{k=1}^{\infty} \bar{w}_k \mu_k.$$

Hierarchical Bayes (continued) VII

- For this particular example, the sum can be calculated exactly. However, we can also approximate this using software by taking the first K partial sums. Check out the provided HB-code R code.

HB Review 3/12

- $\pi_0(\theta)$ - prior, $L(\theta)$ - likelihood.

$$L(\theta) \sim \text{Binomial}(n, \theta)$$

$$\pi_0(\theta) \sim \text{Beta}(\alpha, \beta)$$

↑ ↑
why not random?



$$\begin{aligned}\pi(\theta) &= \int \pi_{\theta, \theta_1}(\theta, \theta_1) d\theta_1 \\ &= \int \pi_{\theta|\theta_1}(\theta|\theta_1) \pi_{\theta_1}(\theta_1) d\theta_1\end{aligned}$$

(1) We want to be "uncommittal" about choice of prior.

$$\pi_{\theta|\theta_1} \sim \text{Beta}(\theta_1, \theta_1)$$

$$E_{\theta|\theta_1}[\theta|\theta_1] = \frac{1}{2}$$

(2) Help w/ integration

Posterior mean =

$$E_{\theta|X}[\theta|X] = \int \theta \pi(\theta|X) d\theta$$

$$E_z[z] = E_Y[E[z|Y]]$$

\swarrow
 z

\swarrow
 Y
 \swarrow
 $Y = \theta|X$

$$\underline{E_{\theta_1 | X}[\theta_1 | X]} = E_{\theta_1 | X}[\underline{E_{\theta_1 | \theta_1, X}[\theta_1 | \theta_1, X]}]$$

• $\theta_1 | \theta_1, X \leftarrow$ easy,

conjugate

$\theta_1 | \theta_1 \sim \underline{\text{Beta}}$

$\theta_1 | \theta_1, X \sim \text{Beta}$

$E[\theta_1 | \theta_1, X] = \underline{\underline{\mu_k}}$, k is value of θ_1

• θ, X

$$\begin{aligned}\pi_{\theta, X}(\theta, X) &\propto \pi_{X|\theta}(X|\theta) \pi_{\theta}(\theta) \\ &= \underline{w_k} -\end{aligned}$$

$$\pi_{\theta, X}(k) = \frac{w_k}{\sum_k w_k}$$

$$E[\theta|X] = \sum \frac{w_k}{\sum_k w_k} \cdot \mu_k$$

In this example:

- (1) • pushed decisions about prior to the "hyper-prior"
- (2) • eased calculations using our designed structure.
- (3) Natural H. Structure.

Baseball statistics

- One place that Hierarchical Bayes is particularly useful is for grouped data:



- Let $i = 1, 2, \dots, k$ denote k distinct groups, and $j = 1, 2, \dots, n_i$ be the number of observations, per each group.
- Then, the data look like:

$$Y_{1,1}, \dots, Y_{1,n_1}, Y_{2,1}, \dots, Y_{2,n_2}, \dots, Y_{k,n_k}$$

- We then have a natural Hierarchical structure to our model, where within each group i , the observations $1, \dots, n_i$ are iid:

$$Y_{i,j} \stackrel{\text{iid}}{\sim} f(y; \theta_i)$$

~~Ridge~~: Standard $\min_{\beta} \frac{1}{n} \sum (y - \hat{y}(\beta))^2$

Ridge: $\min_{\beta} \frac{1}{n} \sum (y - \hat{y}(\beta))^2 + \frac{1}{\lambda} \|\beta\|_2^2$

2000's / 2010's

$\beta_i \sim N(0, \sigma^2)$

MAP (β) \equiv Ridge estimate.

Baseball statistics II

- Then, we create a prior for the group-parameters:

$$\Theta_i \stackrel{\text{iid}}{\sim} \pi(\theta).$$

- This approach is extremely useful as a form of regularization

Baseball: Hitting Percentages

Consider two baseball players, A and B. Player A has a career batting average of 0.353, whereas Player B has an average 0.400. Which do you prefer on your team?

Player A: $\frac{353}{1000}$, Player B: $\frac{4}{10}$

Best hitting average ALL TIME.

• 3662 - Ty Cobb.

≈ 200 players ever have
batted about .300.

(1) group data, penalize towards
know means.

X_A = # of successes for player A.

$$X_A \sim \text{Bin}(1000, p_A)$$

$$\hat{p}_A \approx \frac{353}{1000} \quad (\text{MLE}).$$

$$X_B \sim \text{Bin}(10, p_B)$$

$$\hat{p}_B \approx \frac{4}{10} \quad (\text{MLE})$$

$$P_i \sim B(\alpha, \beta),$$

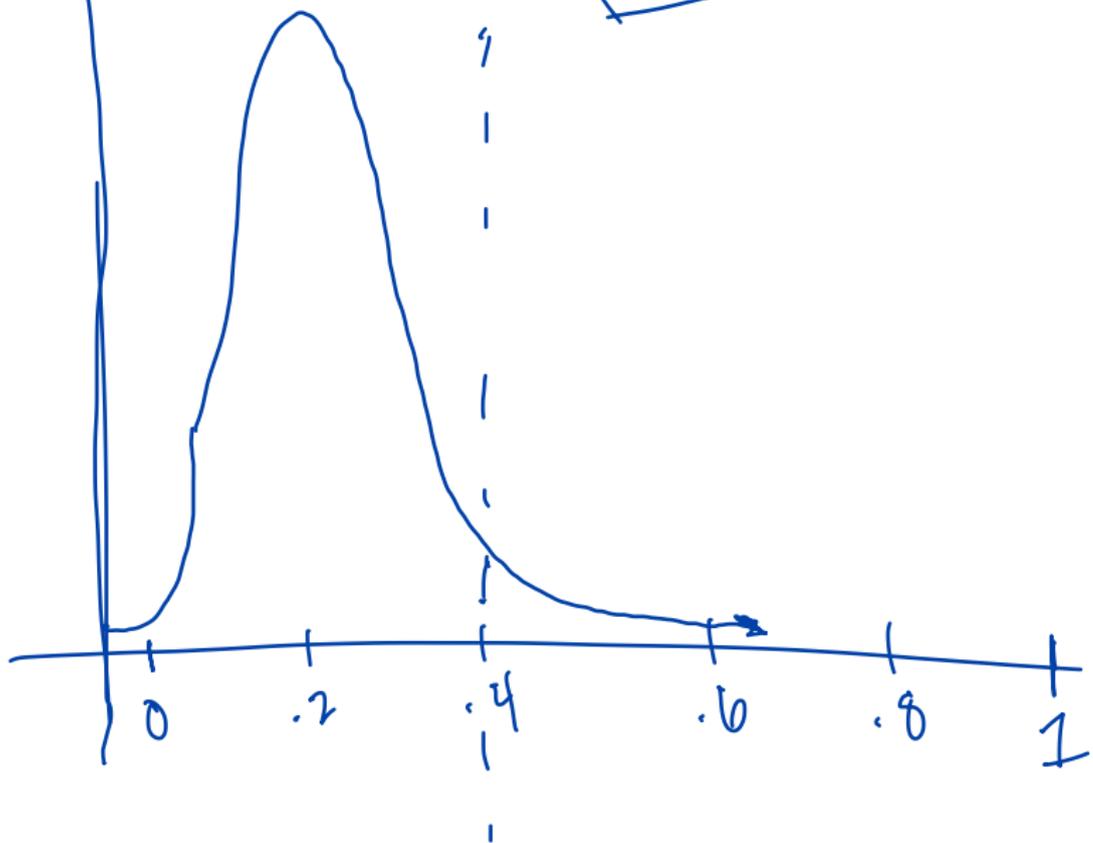
$$\begin{aligned} \bullet E[P_i] &= \underline{0.25}, \\ &= \frac{\alpha}{\alpha + \beta} \Rightarrow \underline{\underline{3\alpha = \beta}}. \end{aligned}$$

$$\bullet 0.25 + 2\sigma = 0.4$$

$$\sigma \approx \frac{15}{200},$$

$$\boxed{\alpha \approx 7}$$

$$\beta = 21$$



$$P_i | X_i = x_i \sim \text{Beta}(\alpha + x_i, \beta + n_i - x_i)$$

$$P_A | X_A = x_A \sim \text{Beta}(7 + 353, 21 + 647)$$

$$P_B | X_B = x_B \sim \text{Beta}(7 + 4, 21 + 6)$$

$$E[P_A | X_A] = \underline{0.350} \quad \left(\underline{0.353} \right)$$

$$E[P_B | X_B] = \underline{0.289} \quad \left(\underline{0.400} \right)$$

$$E[P_B] = \underline{\underline{0.25}}$$

Empirical Bayes

Empirical Bayes

- The idea because Empirical Bayes is simple: Use the data to estimate the prior distribution for the parameters.
- This is a bit controversial, because we're “double dipping”. Often makes sense when used in conjunction with a hierarchical structure.

Empirical Bayes II

Baseball Players

Let's revisit the Baseball-batting percentage problem. Now, we want to estimate the posterior via maximum likelihood of IID Beta distribution, using dataset of historic baseball-player data.

Brad Efron: Didn't like
Bayesians but huge
proponent of E.B.

Uncertainty quantification

Uncertainty in Bayes estimates

- Uncertainty quantification is very natural in Bayesian models.
- We won't focus on too many examples, but will introduce the basic concepts.

Approach 1: Posterior variance

Since our estimates correspond to an entire distribution of $\Theta|X = x^*$, one natural idea is to use the posterior variance to report uncertainty:

$$\text{Var}(\Theta|X = x^*).$$

Uncertainty in Bayes estimates II

Approach 2: quantiles (credible intervals)

Another common approach is to get desired percentiles / quantiles of the posterior. For instance, picking $\alpha = 0.05$, then we might want to select an interval of $I_\alpha = (\theta_{\alpha/2}, \theta_{1-\alpha/2})$ to represent our confidence, where θ_x corresponds to the x th percentile of the posterior. In this case,

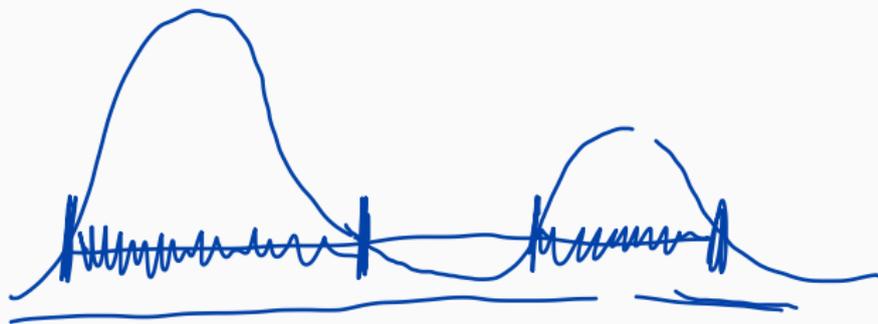
$$\begin{aligned} P(\Theta \in I_\alpha | X = x^*) &= P(\theta_{\alpha/2} \leq \Theta \leq \theta_{1-\alpha/2} | X = x^*) \\ &= F_{\Theta|X}(\theta_{1-\alpha/2}) - F_{\Theta|X}(\theta_{\alpha/2}) \\ &= 1 - \alpha \end{aligned}$$

Uncertainty in Bayes estimates III

Approach 3: high-density region (or high-posterior density)

Also called credible intervals, but constructed in a different way, is the high-density-region (HDR) approach. Here, we take as our set that measures uncertainty the set:

$$R_\alpha(\Theta) = \{\Theta : \pi_{\Theta|X}(\theta|x^*) \geq 1 - \alpha\}.$$



Conclusion

Concluding Remarks

- Bayesian statistics is more than just a philosophy of what probability is, but also a useful way to solve hard problems.
- At the earliest stages of the statistics discipline, most approaches were fundamentally Bayesian, until Fisher in the early 1900s
- The approach lost some popularity until the late 1900s, due to the numeric difficulties that often arise.
- Advances in hardware, software, and methodology caused an explosion of Bayesian statistics research, which continues today.

Concluding Remarks II

- Some of the algorithms that led to this success include:
- Markov-chain Monte Carlo (MCMC) algorithms. Importance sampling is hard in high-dimensions, and often fails in time-series / spatial statistics. Further, a good importance distribution is not always available. MCMC is a class of algorithms that largely solve this issue, by using **dependent** samples; the next sample in a “Chain” is a permutation of previous samples, guided by the likelihood function.
- Sequential Monte Carlo (SMC) algorithms. In many time-series examples, even MCMC fails because of the unique dependence of the model. SMC addresses this by doing Monte-Carlo one step (observation) at a time. The most famous example of this is the **particle filter**.

Concluding Remarks III

- Despite some heated arguments on the topic, a well-done analysis with sufficient data usually result in the same practical solutions, whether a Bayes or Frequentist approach is taken.
- There's somewhat of a general consensus that Bayesian methods are particularly useful when the sample size is small; here, the data alone might not have enough information to tell us about the model, and we benefit from using a prior belief.
- Frequentist methods still dominate in the areas of hypothesis testing, mean comparison, etc.; this is where statistics is used most often by non-statisticians, so it remains the dominant approach in science.

Concluding Remarks IV

- However, there are increasing complaints about the accepted approach (by statisticians and non-statisticians alike), and this has given rise to more Bayesian applications.

References and Acknowledgements

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References and Acknowledgements II

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